

Fundamental Bands of $^{32}\text{S}^{16}\text{O}_2$

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Page	Line	Addenda or Errata
30	footnote f, add	These values have been corrected for hot band contributions in Ref. 31.
31	20	found several relatively
	21 - 22	for example, with observed positions at 543.60, 1132.03
	22	(see Tables III - V)
	24	for some other lines
33	Ref. 24	J. Chem. Phys. <u>58</u> , 265 (1973).
34	Ref. 31	Chem. Phys. Letters, to be published, 1973.
	Ref. 34	W. W. Kellogg
	Ref. 36	J. Chem. Phys. <u>57</u> , 4676 (1972).

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ABSTRACT

The infrared-active vibration-rotation fundamentals of sulfur dioxide have been measured with moderately high spectral resolution. Quantum number assignments have been made for spectral lines from $J = 0$ to 57, by comparison with theoretically computed spectra which include the effects of centrifugal distortion. The following values for the band centers have been determined: $v_1^o = 1151.65 \pm 0.10 \text{ cm}^{-1}$, $v_2^o = 517.75 \pm 0.10 \text{ cm}^{-1}$, and $v_3^o = 1362.00 \pm 0.10 \text{ cm}^{-1}$. Intensities of the observed lines have also been computed. Dipole moment derivatives have been obtained.

I. INTRODUCTION

Nearly twenty years have passed since the important systematic observation of 17 infrared-active vibration-rotation bands of sulfur dioxide by Shelton, Nielsen, and Fletcher.¹ In that work on $^{32}\text{S}^{16}\text{O}_2$, unfavorable energy and detector conditions in several spectral regions necessitated the use of slits ranging from 0.30 to 2.00 cm^{-1} . Consequently, it was not possible to resolve individual transitions, and only sub-branches were assigned.

More recently, high-resolution microwave and far-infrared spectra of SO_2 arising from pure rotational transitions in the ground and excited states have been obtained.²⁻⁷ From analyses of these spectra, accurate values of rotational and centrifugal distortion constants are available. Hinkley *et al.*⁸ have now observed some individual transitions of the v_1 vibration-rotation bands of SO_2 using tunable semiconductor lasers with very high resolution.⁹ Prior to our knowledge of this most recent work,^{8,9} we undertook moderately high-resolution studies of all three infrared-active fundamentals of $^{32}\text{S}^{16}\text{O}_2$ in order to assign as many individual vibration-rotation transitions as possible.

The experimental details for our absorption spectra are discussed in the next Section. In Section III, asymmetric rotor theory is reviewed briefly. Then we present our results in the form of measured spectra, and tabulated experimental and theoretical positions for more than twelve hundred lines. In the last Section, we discuss future studies in which certain experimental and theoretical advances may be expected. Finally, we consider the potential application of our results to laser science and to air pollution problems.

II. EXPERIMENTAL DETAILS

The anhydrous grade $^{32}\text{S}^{16}\text{O}_2$ gas sample was obtained from Matheson Gas Products. The stated purity of the sample was 99.98% by weight; with 50, 10, and 30 p.p.m. maxima of H_2O , H_2SO_4 , and non-volatiles, resp. A Perkin-Elmer Model 225 Grating Infrared Spectrophotometer, equipped with an f/5 fore monochromator for pre-dispersion of the radiation, was

used to record the spectra. A 150 lines/mm grating was employed in the first order for the 1100 to 1400 cm^{-1} region, and a 30 lines/mm grating in the second order for the 475 to 600 cm^{-1} region. A servo-controlled slit program was utilized to provide constant energy to the thermopile detector. A filtered Sola transformer served as a power supply which minimized external electrical noise and provided a constant voltage to the spectrophotometer.

Before each run, the alignment of the Littrow mount in the fore monochromator, and the position of the thermopile relative to the emerging radiation source were precisely adjusted to maximize signal strength. All scans were recorded on a Model 225 Auxiliary Recorder at a speed of $0.5 \text{ cm}^{-1}/\text{min}$ at suitable scale expansions. A minimum of five runs was taken for each vibration-rotation band. The best two runs with respect to reproducibility, resolution, and noise level were selected for the theoretical analysis of each band.

Two 10-cm absorption cells, one with NaCl and the other with KBr windows, were used. The cells were placed in the sample compartment for one hour prior to each run in order to stabilize (at approximately 315°K) the temperature increase caused by heating from the Globar radiation source.

The details of our experimental conditions are summarized in Table I. Several runs of v_2 were also made using cells with KRS-5 windows. However, it was found that substantially higher energy was available with the KBr windows due to their lower refractive index; hence, narrower slits could be used. For calibration purposes, spectra with resolution comparable to that achieved in the present work were chosen. In spite of the larger slit width and lower dispersion in our measurements of v_2 , the absolute accuracy in its line positions is the same as that for v_1 and v_3 because of a better intercomparison with the calibration lines.¹¹

TABLE I
EXPERIMENTAL CONDITIONS

	v_1	v_2	v_3
Pressure (torr)	30	40	1
Temperature ($^{\circ}$ K)	315 ± 5	315 ± 5	315 ± 5
Cell length (cm)	10	10	10
Window material	NaCl	KBr	NaCl
Slit width (cm^{-1}) ^a	0.16 ± 0.02	0.32 ± 0.09	0.17 ± 0.02
Dispersion (cm/cm^{-1}) ^b	2.5	1	2.5
Calibration band	v_2 of NH_3 ^c	v_5 of C_2D_2 ^d	v_4 of CH_4 ^c
Relative accuracy (cm^{-1})	± 0.05	± 0.05	± 0.05
Absolute accuracy (cm^{-1})	± 0.10	± 0.10	± 0.10
Grating (lines/mm)	150	30	150
Grating (order)	first	second	first

^aObtained directly from instrumental readings; errors represent maximum range of values.

^bDetermined from comparisons of SO_2 and calibration lines recorded at identical instrumental settings; errors are less than 1%.

^cFrom Ref. 10.

^dFrom Ref. 11.

III. THEORETICAL ANALYSIS

The sulfur dioxide molecule is an asymmetric rotor with C_{2v} symmetry,¹² whose bond length and bond angle are 1.4308 Å and $119^{\circ}20'$, resp.⁷ As the theory of asymmetric top spectra is well known,^{12,13} only a brief review pertinent to present work will be given. From Kivelson and Wilson's¹⁴ theory for first-order centrifugal distortion, with the inclusion of second-order terms¹⁵ up to $\langle P_z^4 \rangle$, the energy expression is

$$\begin{aligned}
E = E_r - [D_J + 2R_6]J^2(J+1)^2 - [D_{JK} - 4R_6]J(J+1)\langle P_z^2 \rangle \\
- [D_K + 2R_6]\langle P_z^4 \rangle + 2\sigma\delta_J[\langle P_z^2 \rangle - W]J(J+1) \\
+ 4R_5\sigma[\langle P_z^2 \rangle W - \langle P_z^4 \rangle] + 4R_6\sigma^2[\langle P_z^4 \rangle - 2\langle P_z^2 \rangle W + W^2] \\
+ H_{JK}J^2(J+1)^2\langle P_z^2 \rangle + H_{KJ}J(J+1)\langle P_z^4 \rangle,
\end{aligned} \tag{1}$$

where

$$E_r = \frac{1}{2}(B+C)J(J+1) + [A - \frac{1}{2}(B+C)]W(b_p), \tag{2}$$

$$\sigma = -1/b_p = (2A - B - C)/(B-C), \tag{3}$$

and A, B, and C are the rotational constants in order of decreasing magnitude. E_r is the rigid rotor energy and $W \equiv W(b_p)$ is the Wang reduced energy. J is the quantum number corresponding to the total angular momentum operator with molecule-fixed z-component P_z . General formulas for the expectation values $\langle P_z^2 \rangle$ and $\langle P_z^4 \rangle$ have been given in Ref. 14. The D's, R's, and σ_J are linear combinations of the τ 's, coefficients of centrifugal distortion.¹⁴

The absolute intensity of an absorption line corresponding to a transition between initial and final states with quantum numbers n'' and n' , resp., is¹⁶

$$I_{n''n'} = \frac{8\pi^3 N g_{n''} v [1 - \exp(-hv/kT)] \exp(-E_{n''}/kT)}{3hcp \sum_{n''} g_{n''} \exp(-E_{n''}/kT)} \times |\mu_{n''n'}|^2, \tag{4}$$

where N is the number of molecules per cm^{-3} , $v \equiv (E_{n'} - E_{n''})/h$ is the central frequency of the line, and $g_{n''}$ is the statistical weight factor. The quantity $\mu_{n''n'}$ is the expectation value of the transition dipole moment, p and T are the gas pressure and temperature, resp., and k, h, and c are universal constants. Eq. (4) can be simplified by collecting into a single constant C all quantities which are essentially unchanged for all the lines of a particular vibration-rotation band. Also, expressing $|\mu_{n''n'}|^2$ in terms of $S_{R''R}^g$, (the square of the direction cosine matrix element along the molecule-fixed g axis) and dipole-moment derivatives,¹⁷ we obtain for the case of a rigid rotor

$$I_{n''n'}^o = C g_{n''} v_i [1 - \exp(-hv_i/kT)] [\exp(-E_{R''}/kT) \left(\frac{\pi}{4\pi c v_i} \right)^2 \sum_g S_{R''R'}^g \left(\frac{\partial \mu_g}{\partial Q_i} \right)^2], \quad (5)$$

where R represents the rotational quantum numbers, and Q_i is the normal coordinate for the fundamental vibration v_i . The band center is denoted by v_i^o .

For a given fundamental vibration, Eq.(5) reduces further to

$$I_{n''n'}^o = C' g_{n''} \left(\frac{v_i}{v_i^o} \right) [1 - \exp(-hv_i/kT)] [\exp(-E_{R''}/kT) \sum_g S_{R''R'}^g], \quad (6)$$

where

$$C' = \frac{\pi N}{3c^2 p \sum_{n''} g_{n''} \exp(-E_{n''}/kT)} \left[\left(\frac{\partial \mu_a}{\partial Q_i} \right)^2 \text{ or } \left(\frac{\partial \mu_b}{\partial Q_i} \right)^2 \right]. \quad (7)$$

The factorization of Eq.(5) into Eqs.(6) and (7) is a consequence of the fact that the fundamental bands of planar asymmetric rotors such as SO_2 are of only two types. These are denoted by A (as in v_3) or B (as in v_1 and v_2) for which the dipole-moment derivative is along the axis of least (a-axis) or intermediate (b-axis) moment of inertia. Thus

$$\sum_g \left(\frac{\partial \mu_g}{\partial Q_i} \right)^2 = \left(\frac{\partial \mu_a}{\partial Q_i} \right)^2 \text{ or } \left(\frac{\partial \mu_b}{\partial Q_i} \right)^2. \quad (8)$$

For computing line intensities $I_{n''n'}^o/C'$ and line positions $(E_{n''} - E_{n'})/h$, we have used the computer program originally written by Pierce and modified by Eggers.¹⁸ This program is very compact and fast.¹⁹ In it, the wave-number range of the entire band is divided into a large number of intervals, each of which may be taken as approximately half a resolution element. The intensity of each transition is assigned to the appropriate interval. When these assignments are completed, the intensity in each interval is distributed over adjacent intervals according to a Gaussian function which takes into account the finite width of the absorption lines. We have used, instead, a triangular distribution function with base equal to twice our experimental slit width. We found that this approach gave the best

TABLE II
ROTATIONAL AND CENTRIFUGAL DISTORTION CONSTANTS FOR $^{32}\text{S}^{16}\text{O}_2$

<u>Ground State^a</u>		<u>Excited States^c</u>	
Constant	Value (in cm^{-1})	Constant	Value (in cm^{-1})
A	2.0273555 ± 0.0000006		
B	0.3441702 ± 0.0000002		
C	0.2935302 ± 0.0000001	A	2.0284336
τ_{zzzz}	$(-3.3095 \pm 0.0010) \times 10^{-4}$	B	0.3425071
τ_{xxzz}	$(+0.1439 \pm 0.0002) \times 10^{-4}$	C	0.2921169
τ_{xzxz}	$(-0.01775 \pm 0.00018) \times 10^{-4}$		
τ_{xxxx}	$(-0.01331 \pm 0.00003) \times 10^{-4}$		
H_{KJ}	$(-0.0311 \pm 0.0128) \times 10^{-8}$		
H_{JK}	$(-0.0111 \pm 0.0029) \times 10^{-8}$	A	2.0665828
τ_{yyyy}	$- 0.004108 \times 10^{-4}$	B	0.3442469
τ_{yyxx}	$- 0.006665 \times 10^{-4}$	C	0.2930009
τ_{yyzz}	$+ 0.03529 \times 10^{-4}$		
D_J	$+0.0020495 \times 10^{-4}$		
D_K	$+0.865348 \times 10^{-4}$	A	2.0066777
D_{JK}	$-0.0400224 \times 10^{-4}$	B	0.3430118
R_5	$+0.0048567 \times 10^{-4}$	C	0.2924378
R_6	$-0.0063875 \times 10^{-6}$		
δ_J	$+0.00575125 \times 10^{-5}$		
σ	67.47651 ^b		

^aThe first nine values are taken from Ref. 4, the next three are calculated from Eqs. (9-11) of Ref. 15, and the remaining seven are calculated from relations (36) of Ref. 14.

^bDimensionless, see Eq. (3).

^cThe values for v_1 are taken from Ref. 6, and those for v_2 and v_3 are taken from Ref. 2.

agreement between the calculated theoretical spectrum and the overall detailed appearance of our experimental spectrum.

Rotational and centrifugal distortion constants, in the ground and excited vibrational states of SO_2 , used in the computer program have been taken from far-infrared⁴ and microwave^{2,6} spectra. These values and the remaining derived values, calculated from the relations in Refs. 14 and 15, are given in Table II. The computer program takes into account the fact that in the ground state of SO_2 only symmetric levels occur because of C_{2v} symmetry and zero spin of the ^{16}O nuclei. The initial values for the three band centers were taken from the work of Shelton *et al.*¹. These values were later adjusted so that the experimental and theoretical spectra would match.

The dipole moment derivatives for the fundamentals were calculated in the following way. Equation (6) was summed over all transitions having $J \leq 60$. Previously measured experimental band intensities,²⁰⁻²³ and a projected value,⁸ were taken for $\sum_{n''} I^o_{n''n''}$. Our calculated line intensities were used for the sum on the right-hand side of Eq.(6), so that C' was determined. The sum over n'' in Eq.(7) could be factored, to a good approximation, into a vibrational and a rotational partition function which were readily evaluated from Eqs.(V,17) and (V,29), resp., of Ref. 12. Finally, from the value of C' obtained using Eq.(6), the dipole moment derivatives were deduced from Eq.(7). As the derivatives occur squared in Eq.(7), only their absolute values could be determined by this method.

IV. RESULTS

The results of our experimental and theoretical studies of the fundamental infrared bands of $^{32}\text{S}^{16}\text{O}_2$ are summarized in Figs. 1-3 and Tables III-VI. A representative portion of these results have also been presented in Ref. 24. The experimental conditions were given in Table I. Spectral resolution in the $1100-1400 \text{ cm}^{-1}$ region for ν_1 and ν_3 was typically about 0.12 cm^{-1} , with isolated instances of 0.10 cm^{-1} or better. In the $475-600 \text{ cm}^{-1}$ region for ν_2 , resolution was characteristically 0.25 cm^{-1} , and occasionally 0.20 cm^{-1} or better. In the Figures, the upper tracings are the measured experimental spectra, with percent absorption shown in the right-hand vertical scales. It should be noted that both the measured spectra and the right-hand scales are displaced upward by the same amount,

so that 0% absorption denotes the experimental base line.

Our calculated theoretical spectra are also represented in Figs. 1-3. These spectra are the lower tracings, with relative intensity on the left-hand vertical scales. The intensity plotted in the Figures is a normalized distribution of line intensities. This distribution into small intervals was discussed in Sec. III. The normalization, on a linear scale, is made with respect to that distribution of intensities (arbitrarily assigned the value 100 for v_1 and v_3 , and 90 for v_2) which is the maximum for all the intervals in a given band. As can be seen in the Figures, there is good agreement between the theoretical and experimental spectra.

In Tables III-V, the observed and computed spectral line positions are compared. Only the stronger theoretical transitions corresponding to each experimental line peak have been listed in these Tables. (Where there is a blank space in the column of experimental line positions, the adjacent theoretical line position corresponds to the previously tabulated experimental line.) With very few minor exceptions, 97% of the tabulated computed lines fall within $\pm 0.05 \text{ cm}^{-1}$ of the observed lines. Initial- and final-state quantum number assignments, as well as theoretical line intensities $I_{n''n'}^{\circ}/C'$ defined by Eq.(6), are given for the computed lines in Tables III-V. The quantum numbers K_{-1} and K_1 are associated with the projection of the total angular momentum (having quantum number J) on the symmetry axis in, resp., the prolate and oblate symmetric top limiting cases.^{12,13}

Experimental and theoretical results for v_1 in the spectral range from 1112.5 to 1200.0 cm^{-1} are represented in Fig. 1 and Table III. The selection rules²⁵ are $\Delta J = 0, \pm 1$; $J = 0 \leftrightarrow J = 0$; and $\Delta K_{-1} = \pm 1, \pm 3, \dots$. Approximately 450 observed lines have now been assigned. The band center for v_1 has been determined in the present work to be $1151.65 \pm 0.10 \text{ cm}^{-1}$. Earlier infrared observations yielded the values 1152 (Ref. 26), 1151.38 (Refs. 27 and 1), 1152 ± 1 (Ref. 28), and $1151.2 \pm 0.2 \text{ cm}^{-1}$ (Ref. 29). Most recently, Hinkley et al.,⁸ using very high resolution (line width less than 10^{-5} cm^{-1}) techniques, have found a value of $1151.71 \pm 0.01 \text{ cm}^{-1}$ in excellent agreement with our result, to within our experimental error. We have also compared our calculated line positions, taking into account the 0.06 cm^{-1} difference in band centers, to the several rather isolated

TABLE III

COMPARISON OF EXPERIMENTAL AND THEORETICAL SPECTRAL LINE POSITIONS, WITH QUANTUM NUMBER ASSIGNMENTS, FOR THE v_1 BAND OF $^{32}\text{S}^{16}\text{O}_2$ CENTERED AT $1151.65 \pm 0.10 \text{ cm}^{-1}$.
LINE INTENSITIES [SEE SEC.III, ESPECIALLY EQ. (6)] ARE COMPUTED AT 300°K .

Line Position (in cm^{-1})		Quantum Numbers								Line Position (in cm^{-1})		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$		
1112.68	1112.70	29	5	25	30	6	24	1.5189		1119.77	9	7	3	10	8	2	3.6800		
1112.77	1112.80	24	6	18	25	7	19	2.1767	1120.06	1120.04	24	4	20	25	5	21	2.1291		
1112.96	1112.94	19	7	13	20	8	12	2.7233	1120.34	1120.35	18	5	13	19	6	14	2.9815		
1113.07	1113.07	14	8	6	15	9	7	3.1098	1120.44	1120.41	13	6	8	14	7	7	3.4418		
1113.17	1113.17	9	9	1	10	10	0	3.3979		1120.44	8	7	1	9	8	2	3.7582		
1113.48	1113.50	23	6	18	24	7	17	2.3113	1120.59	1120.56	25	3	23	26	4	22	1.3955		
1113.66	1113.63	18	7	11	19	8	12	2.8427	1120.77	1120.73	46	0	46	47	1	47	1.6644		
1113.79	1113.76	13	8	6	14	9	5	3.2075	1120.99	1120.94	38	8	30	38	9	29	1.0263		
1113.87	1113.87	41	10	32	41	11	31	0.5309		1121.04	17	5	13	18	6	12	3.1023		
1114.06	1114.11	27	5	23	28	6	22	1.7850	1121.09	1121.09	12	6	6	13	7	7	3.5155		
1114.17	1114.20	22	6	16	23	7	17	2.4453		1121.10	7	7	1	8	8	0	3.8452		
1114.28	1114.33	17	7	11	18	8	10	2.9578	1121.21	1121.23	22	4	18	23	5	19	2.4065		
1114.40	1114.44	12	8	4	13	9	5	3.3020	1121.38	1121.37	33	8	26	33	9	25	1.5005		
1114.58	1114.61	34	10	24	34	11	23	0.9517	1121.55	1121.51	44	1	43	45	2	44	1.5687		
1114.77	1114.71	33	10	24	33	11	23	1.0171	1121.75	1121.72	16	5	11	17	6	12	3.1934		
1114.85	1114.89	26	5	21	27	6	22	1.9247		1121.76	11	6	6	12	7	5	3.5817		
1114.90	1114.90	21	6	16	22	7	15	2.5771	1121.94	1121.95	38	3	35	39	4	36	1.1678		
1114.98	1115.02	16	7	9	17	8	10	3.0674	1122.11	1122.08	24	8	16	24	9	15	2.2396		
1115.08	1115.11	11	8	4	12	9	3	3.3934		1122.15	23	8	16	23	9	15	2.2793		
1115.28	1115.25	27	10	18	27	11	17	1.3696	1122.59	1122.56	16	8	8	16	9	7	2.0485		
1115.50	1115.51	25	5	21	26	6	20	2.0607		1122.61	15	8	8	15	9	7	1.9208		
1115.57	1115.59	20	6	14	21	7	15	2.7059	1122.83	1122.86	43	1	43	44	0	44	2.3009		
1115.69	1115.71	15	7	9	16	8	8	3.1714	1123.08	1123.09	14	5	9	15	6	10	3.3624		
1115.82	1115.79	10	8	2	11	9	3	3.4844		1123.10	9	6	4	10	7	3	3.6957		
1115.91	1115.89	18	10	8	18	11	7	1.3601	1123.53	1123.48	40	2	38	41	3	39	1.6539		
1115.95	1115.95	17	10	8	17	11	7	1.2821		1123.57	42	0	42	43	1	43	2.5460		
1116.27	1116.24	24	5	19	25	6	20	2.2012	1123.80	1123.77	13	5	9	14	6	8	3.4379		
	1116.29	19	6	14	20	7	13	2.8305		1123.77	8	6	2	9	7	3	3.7491		
1116.47	1116.46	9	8	2	10	9	1	3.5768	1124.13	1124.13	44	7	37	44	8	36	0.6816		
1116.97	1116.98	18	6	12	19	7	13	2.9500	1124.31	1124.27	41	1	41	42	0	42	2.8072		
1117.05	1117.07	13	7	7	14	8	6	3.3608		1124.32	40	1	39	41	2	40	2.3157		
1117.16	1117.13	8	8	0	9	9	1	3.6753	1124.41	1124.44	7	6	2	8	7	1	3.8059		
1117.59	1117.61	22	5	17	23	6	18	2.4758		1124.44	12	5	7	13	6	8	3.4980		
1117.71	1117.67	17	6	12	18	7	11	3.0635	1124.57	1124.61	39	3	37	40	2	38	1.7928		
	1117.75	12	7	5	13	8	6	3.4463	1124.76	1124.77	38	2	36	39	3	37	1.9297		
1118.01	1118.00	28	4	24	29	5	25	1.5874	1124.98	1124.97	40	0	40	41	1	41	3.0845		
1118.12	1118.11	32	9	23	32	10	22	1.3260	1125.14	1125.10	6	6	0	7	7	1	3.8752		
1118.34	1118.31	21	5	17	22	6	16	2.6091		1125.14	11	5	7	12	6	6	3.5581		
	1118.36	16	6	10	17	7	11	3.1700	1125.36	1125.35	25	7	19	25	8	18	2.6148		
1118.48	1118.43	11	7	5	12	8	4	3.5272	1125.46	1125.42	24	7	17	24	8	16	2.6826		
1118.65	1118.62	26	9	17	26	10	16	1.7482		1125.48	23	7	17	23	8	16	2.7364		
	1118.70	25	9	17	25	10	16	1.7966	1125.60	1125.55	22	7	15	22	8	14	2.7744		
1119.02	1118.98	20	5	15	21	6	16	2.7392		1125.61	21	7	15	21	8	14	2.7944		
	1119.05	15	6	10	16	7	9	3.2690	1125.69	1125.67	39	1	39	40	0	40	3.3775		
1119.30	1119.27	16	9	7	16	10	6	1.5863	1125.83	1125.79	10	5	5	11	6	6	3.5865		
	1119.32	15	9	7	15	10	6	1.4597		1125.88	16	7	9	16	8	8	2.5607		
1119.38	1119.37	14	9	5	14	10	4	1.3056	1126.06	1126.02	13	7	7	13	8	6	2.0840		
	1119.41	13	9	5	13	10	4	1.1210		1126.06	12	7	5	12	8	4	1.8561		
1119.62	1119.66	19	5	15	20	6	14	2.8635	1126.14	1126.13	19	3	17	20	4	16	2.4674		
1119.73	1119.73	14	6	8	15	7	9	3.3595	1126.37	1126.37	38	0	38	39	1	39	3.6848		

TABLE III (Continued)

Line Position (in cm ⁻¹)		Quantum Numbers								Line Positions (in cm ⁻¹)		Quantum Numbers							
Exptl.	Theor.	J'	K' ₋₁	K' ₁	J''	K'' ₋₁	K'' ₁	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K' ₋₁	K' ₁	J''	K'' ₋₁	K'' ₁	$\frac{I^o}{C'}$		
1126.45	1126.46	9	5	5	10	6	4	3.6173	1132.37	1132.32	28	1	27	29	2	28	4.9822		
1126.60	1126.61	44	1	43	44	2	42	0.5291		1132.37	21	5	17	21	6	16	3.8563		
1126.72	1126.74	20	3	17	21	4	18	2.5034		1132.42	20	5	15	20	6	14	3.8760		
1127.08	1127.06	37	1	37	38	0	38	4.0059	1132.57	1132.55	17	5	13	17	6	12	3.7769		
	1127.12	8	5	3	9	6	4	3.6422		1132.60	16	5	11	16	6	10	3.6857		
1127.71	1127.75	36	0	36	37	1	37	4.3388	1132.67	1132.64	15	5	11	15	6	10	3.5412		
1128.15	1128.14	32	2	30	33	3	31	2.6734		1132.68	14	5	9	14	6	8	3.4059		
	1128.15	35	6	30	35	7	29	1.8199		1132.71	13	5	9	13	6	8	3.2143		
1128.25	1128.27	33	6	28	33	7	27	2.0920	1132.91	1132.87	8	5	3	8	6	2	1.7618		
	1128.29	34	6	28	34	7	27	1.9569		1132.88	18	2	16	19	3	17	2.8849		
1128.41	1128.37	32	6	26	32	7	25	2.2303		1132.89	7	5	3	7	6	2	1.1855		
	1128.39	31	6	26	31	7	25	2.3657		1132.96	29	3	27	30	2	28	2.8422		
	1128.44	35	1	35	36	0	36	4.6825	1133.09	1133.13	4	4	0	5	5	1	3.4208		
	1128.45	6	5	1	7	6	2	3.6888	1133.19	1133.17	28	0	28	29	1	29	7.1542		
1128.51	1128.49	11	4	8	12	5	7	3.4145		1133.21	9	3	7	10	4	6	3.1590		
1128.67	1128.63	27	6	22	27	7	21	2.8713	1133.34	1133.31	13	2	12	14	3	11	2.4385		
	1128.69	26	6	20	26	7	19	2.9794	1133.44	1133.48	27	2	26	28	1	27	5.1379		
1128.76	1128.74	25	6	20	25	7	19	3.0759	1133.55	1133.53	26	1	25	27	2	26	5.2657		
	1128.80	24	6	18	24	7	17	3.1595		1133.57	16	2	14	17	3	15	2.8738		
1129.01	1128.97	21	6	16	21	7	15	3.3104	1133.84	1133.85	27	1	27	28	0	28	7.4758		
	1129.02	20	6	14	20	7	13	3.3208	1134.01	1133.98	35	4	32	35	5	31	2.2929		
1129.09	1129.08	19	6	14	19	7	13	3.3080	1134.32	1134.32	35	3	33	35	4	32	2.1068		
	1129.10	5	5	1	6	6	0	3.7091		1134.36	14	2	12	15	3	13	2.8689		
	1129.12	34	0	34	35	1	35	5.0338	1134.42	1134.47	33	4	30	33	5	29	2.6879		
1129.21	1129.16	10	4	6	11	5	7	3.4337	1134.57	1134.54	7	3	5	8	4	4	3.0191		
	1129.23	33	2	32	34	1	33	3.9284	1134.67	1134.66	24	1	23	25	2	24	5.4181		
1129.32	1129.27	15	6	10	15	7	9	2.9860	1134.82	1134.86	31	4	28	31	5	27	3.0826		
	1129.31	14	6	8	14	7	7	2.8287	1134.92	1134.95	25	2	24	26	1	25	5.3532		
	1129.35	13	6	8	13	7	7	2.6368	1135.14	1135.18	25	1	25	26	0	26	8.0512		
1129.40	1129.39	12	6	6	12	7	5	2.4081	1135.23	1135.20	6	3	3	7	4	4	3.0408		
	1129.43	11	6	6	11	7	5	2.1399		1135.26	12	2	10	13	3	11	2.8578		
1129.48	1129.46	10	6	4	10	7	3	1.8285	1135.34	1135.31	33	3	31	33	4	30	2.5510		
	1129.49	9	6	4	9	7	3	1.4691		1135.38	27	4	24	27	5	23	3.8003		
1129.60	1129.58	40	1	39	40	2	38	0.8816		1135.39	31	2	30	31	3	29	2.3144		
1129.75	1129.77	32	1	31	33	2	32	4.1613	1135.52	1135.56	25	4	22	25	5	21	4.0872		
1129.83	1129.81	33	1	33	34	0	34	5.3914	1135.65	1135.69	23	4	20	23	5	19	4.3029		
	1129.83	9	4	6	10	5	5	3.4519	1135.80	1135.76	28	0	28	28	1	27	1.6375		
1130.01	1130.01	14	3	11	15	4	12	3.0600		1135.80	24	0	24	25	1	25	8.2956		
1130.48	1130.48	32	0	32	33	1	33	5.7515	1135.96	1135.95	20	4	16	20	5	15	4.4697		
	1130.49	8	4	4	9	5	5	3.4370	1136.17	1136.16	11	4	8	11	5	7	3.3022		
1130.61	1130.63	31	2	30	32	1	31	4.3889	1136.44	1136.48	23	2	22	24	1	23	5.4102		
1130.69	1130.68	41	5	37	41	6	36	1.2360	1136.51	1136.51	23	1	23	24	0	24	8.5048		
1131.12	1131.07	30	1	29	31	2	30	4.6025	1136.60	1136.58	29	2	28	29	3	27	2.7615		
	1131.12	24	2	22	25	3	23	2.9581	1136.84	1136.87	30	4	26	30	5	25	3.5014		
	1131.17	31	1	31	32	0	32	6.1118	1136.94	1136.95	29	3	27	29	4	26	3.5089		
1131.25	1131.27	12	3	9	13	4	10	3.1494	1137.05	1137.04	25	3	23	26	2	24	2.7784		
1131.48	1131.48	15	2	14	16	3	13	2.1278		1137.09	22	0	22	23	1	23	8.6727		
1131.60	1131.55	35	5	31	36	6	30	2.1061	1137.26	1137.31	32	4	28	32	5	27	3.2221		
1131.69	1131.69	22	2	20	23	3	21	2.9339	1137.41	1137.42	8	2	6	9	3	7	2.7337		
1131.81	1131.83	30	0	30	31	1	31	6.4680		1137.44	30	1	29	30	2	28	2.6369		
1131.90	1131.87	11	3	9	12	4	8	3.1641	1137.51	1137.53	18	1	17	19	2	18	4.9322		
1132.03	1131.98	29	5	25	29	6	24	3.0515	1137.66	1137.69	27	2	26	27	3	25	3.2391		
	1132.03	39	3	37	39	4	36	1.3610	1137.81	1137.83	21	1	21	22	0	22	8.7953		
	1132.04	29	2	28	30	1	29	4.8037	1137.92	1137.88	7	2	6	8	3	5	2.6373		
1132.24	1132.19	25	5	21	25	6	20	3.5706	1138.12	1138.10	21	2	20	22	1	21	5.2795		
	1132.21	26	5	21	26	6	20	3.4612		1138.15	36	4	32	36	5	31	2.6508		
	1132.27	24	5	19	24	6	18	3.6708	1138.32	1138.33	16	1	15	17	2	16	4.5275		
	1132.28	23	5	19	23	6	18	3.7510	1138.35	20	0	20	21	1	21	8.8682			

TABLE III (Continued)

Line Position (in cm ⁻¹)		Quantum Numbers								Line Position (in cm ⁻¹)		Quantum Numbers							
Exptl.	Theor.	J'	K' ₋₁	K' ₁	J''	K'' ₋₁	K'' ₁	$\frac{I^o}{n''n'}$	Exptl.	Theor.	J'	K' ₋₁	K' ₁	J''	K'' ₋₁	K'' ₁	$\frac{I^o}{n''n'}$		
1138.41	1138.42	34	2	32	34	3	31	2.6986	1145.76	1145.72	7	1	7	7	2	6	2.9065		
1138.67	1138.64	6	2	4	7	3	5	2.5886	1145.78	1145.78	18	1	17	18	2	16	7.6320		
	1138.71	25	2	24	25	3	23	3.7254	1146.07	1146.08	6	0	6	7	1	7	4.0047		
1138.84	1138.85	21	3	19	21	4	18	4.9279		1146.10	1146.10	5	1	5	5	2	4	2.2487	
1139.14	1139.09	19	3	17	19	4	16	5.0126	1146.29	1146.25	16	4	12	15	5	11	1.1381		
	1139.11	14	1	13	15	2	14	4.0803		1146.29	1146.29	27	5	23	28	4	24	1.1181	
	1139.15	19	1	19	20	0	20	8.8828	1146.39	1146.36	3	1	3	3	2	2	1.3572		
1139.52	1139.48	13	3	11	13	4	10	4.3838		1146.43	1146.43	22	5	17	21	6	16	1.0973	
	1139.55	11	3	9	11	4	8	3.8750	1146.62	1146.59	2	1	1	2	2	0	0.8270		
1139.61	1139.59	18	0	18	19	1	19	8.8436	1146.81	1146.84	17	4	14	16	5	11	1.1990		
	1139.65	7	3	5	7	4	4	2.4019	1146.99	1147.02	21	4	18	22	3	19	1.5497		
1139.85	1139.85	18	3	15	18	4	14	5.1505	1147.09	1147.05	12	0	12	12	1	11	5.1220		
1140.03	1140.03	32	2	30	32	3	29	3.4571		1147.12	1147.12	12	1	11	12	2	10	7.4668	
	1140.07	27	4	24	28	3	25	1.4616	1147.16	1147.16	10	1	9	10	2	8	6.3111		
1140.42	1140.42	21	2	20	21	3	19	4.5928	1147.46	1147.47	7	2	6	6	3	3	0.6133		
	1140.44	22	3	19	22	4	18	5.3365		1147.50	1147.50	18	4	14	17	5	13	1.2488	
1140.55	1140.55	3	2	2	4	3	1	2.3031	1147.68	1147.67	7	7	1	8	0	8	4.0908		
1140.70	1140.73	26	1	25	26	2	24	3.9157	1147.81	1147.83	15	3	13	16	2	14	1.8796		
1141.01	1141.03	19	1	19	19	2	18	3.0150	1148.03	1148.01	10	0	10	10	1	9	5.5528		
1141.11	1141.10	19	2	18	19	3	17	4.8900		1148.05	1148.05	19	4	16	18	5	13	1.2823	
1141.20	1141.18	26	3	23	26	4	22	5.2910	1148.18	1148.17	2	0	2	3	1	3	1.9475		
	1141.20	2	2	0	3	3	1	2.2393		1148.21	1148.21	25	5	21	24	6	18	1.0752	
1141.38	1141.37	32	3	29	32	4	28	4.3161	1148.28	1148.28	25	5	21	26	4	22	1.2159		
1141.48	1141.44	30	2	28	30	3	27	4.3615	1148.49	1148.48	26	5	21	27	4	24	1.1349		
	1141.44	28	3	25	28	4	24	5.1249	1148.61	1148.58	14	3	11	13	4	10	1.2668		
1141.53	1141.53	30	3	27	30	4	26	4.8040	1148.75	1148.75	8	0	8	8	1	7	5.6104		
1141.84	1141.85	15	1	15	16	0	16	8.3027		1148.77	1148.77	20	4	16	19	5	15	1.3084	
1141.93	1141.94	14	0	14	15	1	15	8.0252	1148.87	1148.88	26	5	21	25	6	20	1.0533		
1142.10	1142.08	17	1	17	17	2	16	3.2916	1148.98	1148.97	9	2	8	10	1	9	1.9883		
	1142.11	15	2	14	15	3	13	5.0050	1149.18	1149.18	5	1	5	6	0	6	2.8037		
1142.33	1142.37	24	1	23	24	2	22	4.7593	1149.27	1149.29	6	0	6	6	1	5	5.1109		
1142.43	1142.46	13	2	12	13	3	11	4.7709	1149.41	1149.40	27	5	23	26	6	20	1.0221		
1142.52	1142.53	6	1	5	7	2	6	2.3426	1149.72	1149.72	11	2	10	10	3	7	1.1804		
1142.72	1142.71	11	2	10	11	3	9	4.3361	1149.83	1149.86	2	0	2	2	1	1	2.4036		
1143.00	1143.00	7	2	6	7	3	5	2.9282	1150.16	1150.14	17	3	15	16	4	12	1.4377		
	1143.03	15	1	15	15	2	14	3.5021	1150.26	1150.28	16	3	13	17	2	16	1.2610		
	1143.04	12	0	12	13	1	13	7.2264	1150.72	1150.73	7	2	6	8	1	7	1.4153		
1143.12	1143.12	18	0	18	18	1	17	3.4440	1150.88	1150.90	17	4	14	18	3	15	1.5217		
	1143.17	8	2	6	8	3	5	3.4007	1151.09	1151.11	14	3	11	15	2	14	1.3597		
1143.22	1143.24	13	1	13	14	0	14	7.5874	1151.24	1151.22	19	3	17	18	4	14	1.4650		
1143.34	1143.30	10	2	8	10	3	7	4.2219		1151.26	1151.26	12	2	10	11	3	9	1.4125	
1143.54	1143.50	12	2	10	12	3	9	4.9900	1151.45	1151.45	18	3	15	17	4	14	1.5178		
	1143.56	4	1	3	5	2	4	1.9394	1151.55	1151.54	15	2	14	14	3	11	1.3504		
1143.76	1143.78	14	2	12	14	3	11	5.7326		1151.57	1151.57	25	4	22	24	5	19	1.2357	
	1143.79	3	1	3	4	2	2	1.5901	1152.02	1152.06	1	1	1	2	0	2	0.5152		
1143.88	1143.88	13	1	13	13	2	12	3.6079	1152.20	1152.16	17	2	16	16	3	13	1.2543		
1144.08	1144.03	24	2	22	24	3	21	7.0346		1152.21	1152.21	21	3	19	20	4	16	1.4165	
	1144.06	16	2	14	16	3	13	6.4419	1152.40	1152.39	8	1	7	7	2	6	1.4213		
1144.27	1144.30	18	2	16	18	3	15	7.0459		1152.40	1152.40	5	2	4	6	1	5	0.8794	
1144.37	1144.34	22	2	20	22	3	19	7.4290	1152.53	1152.52	19	2	18	18	3	15	1.0645		
	1144.41	20	2	18	20	3	17	7.4164	1152.62	1152.60	4	0	4	3	1	3	1.6167		
1144.64	1144.61	11	1	11	11	2	10	3.5673		1152.66	1152.66	27	4	24	26	5	21	1.1383	
	1144.68	11	1	11	12	0	12	6.5969	1152.75	1152.79	20	5	15	21	4	18	1.3376		
1144.82	1144.84	20	1	19	20	2	18	6.7459	1153.05	1153.01	26	4	22	25	5	21	1.2263		
1145.08	1145.08	8	0	8	9	1	9	5.1188		1153.06	1153.06	20	3	17	19	4	16	1.5669	
1145.28	1145.27	9	1	9	9	2	8	3.3423	1153.21	1153.24	10	3	7	11	2	10	1.1990		
	1145.29	13	2	12	14	1	13	3.2313	1153.32	1153.30	9	3	7	10	2	8	1.1368		
1145.63	1145.62	15	4	12	14	5	9	1.0631	1153.46	1153.43	2	1	1	2	0	2	2.4317		

TABLE III (Continued)

Line Position		Quantum Numbers								Line Position		Quantum Numbers							
		(in cm ⁻¹)										(in cm ⁻¹)							
Exptl.	Theor.	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\frac{I^o}{C'}$		Exptl.	Theor.	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\frac{I^o}{C'}$	
1153.57	1153.60	4	1	3	4	0	4	4.0585		1161.46	1161.48	9	2	8	8	1	7	2.9454	
1153.68	1153.68	14	4	10	15	3	13	1.3623		1161.65	1161.67	17	1	17	16	0	16	9.1805	
1153.87	1153.89	6	1	5	6	0	6	5.1828		1161.79	1161.75	28	2	26	28	1	27	3.4262	
1153.99	1154.01	6	0	6	5	1	5	2.8458		1161.96	1161.94	20	4	16	20	3	17	5.6210	
	1154.03	10	1	9	9	2	8	2.0182		1162.24	1162.23	11	2	10	10	1	9	3.4213	
1154.22	1154.18	13	4	10	14	3	11	1.2948		1162.58	1162.55	36	3	33	36	2	34	2.2427	
	1154.24	18	5	13	19	4	16	1.3158		1162.71	1162.67	19	1	19	18	0	18	9.5430	
1154.32	1154.33	8	1	7	8	0	8	5.7021			1162.73	4	3	1	3	2	2	2.4772	
1154.48	1154.45	8	3	5	9	2	8	0.9528			1162.75	32	5	27	32	4	28	3.4451	
1154.81	1154.82	22	3	19	21	4	18	1.5819		1162.97	1162.97	23	2	22	23	1	23	2.5725	
1154.92	1154.90	17	5	13	18	4	14	1.2858			1162.99	20	0	20	19	1	19	9.6043	
	1154.96	10	1	9	10	0	10	5.6626		1163.08	1163.07	30	2	28	30	1	29	2.8387	
1155.10	1155.10	3	1	3	2	0	2	1.9924			1163.10	19	4	16	19	3	17	5.3980	
1155.47	1155.44	8	0	8	7	1	7	4.1914		1163.36	1163.32	13	4	10	13	3	11	4.7295	
1155.77	1155.75	14	2	12	14	1	13	8.3110			1163.34	5	3	3	4	2	2	2.5867	
	1155.81	10	2	8	10	1	9	6.4671			1163.36	27	3	25	27	2	26	3.5012	
1155.96	1156.00	16	2	14	16	1	15	8.3573		1163.48	1163.45	27	4	24	27	3	25	4.2901	
1156.25	1156.28	6	2	4	6	1	5	3.5471			1163.51	15	2	14	14	1	13	4.4284	
1156.52	1156.52	4	2	2	4	1	3	2.1798		1163.67	1163.68	21	1	21	20	0	20	9.6395	
	1156.55	18	2	16	17	3	15	2.1532		1164.12	1164.08	22	0	22	21	1	21	9.5864	
1156.78	1156.78	14	1	13	14	0	14	4.6794			1164.09	17	2	16	16	1	15	4.9375	
1156.88	1156.85	10	0	10	9	1	9	5.5801		1164.36	1164.35	28	5	23	28	4	24	4.0897	
	1156.92	3	2	2	3	1	3	1.4049		1164.52	1164.54	7	3	5	6	2	4	2.8192	
1157.09	1157.08	7	1	7	6	0	6	4.1544		1164.71	1164.68	19	2	18	18	1	17	5.4038	
	1157.12	5	2	4	5	1	5	2.3308			1164.69	23	1	23	22	0	22	9.4980	
1157.38	1157.38	22	3	19	22	2	20	7.6736		1164.98	1164.98	26	5	21	26	4	22	4.3905	
	1157.39	24	3	21	24	2	22	7.2681		1165.08	1165.10	24	1	23	23	2	22	5.9336	
	1157.42	14	1	13	13	2	12	3.3537		1165.18	1165.14	24	0	24	23	1	23	9.3436	
1157.56	1157.58	20	3	17	20	2	18	7.6701			1165.20	35	4	32	35	3	33	3.2080	
1157.69	1157.66	26	3	23	26	2	24	6.5140		1165.34	1165.32	21	2	20	20	1	19	5.7718	
1157.89	1157.93	16	1	15	16	0	16	4.1120			1165.37	24	5	19	24	4	20	4.6456	
1158.05	1158.08	22	2	20	22	1	21	5.9510		1165.50	1165.52	35	5	31	35	4	32	2.5137	
1158.20	1158.18	28	3	25	28	2	26	5.5542		1165.73	1165.71	25	1	25	24	0	24	9.1533	
	1158.20	12	0	12	11	1	11	6.8886		1165.82	1165.83	25	5	21	25	4	22	4.4831	
1158.41	1158.41	16	3	13	16	2	14	6.7027			1165.86	22	5	17	22	4	18	4.8266	
1158.63	1158.62	32	4	28	32	3	29	4.4930		1165.93	1165.97	28	2	26	27	3	25	3.1423	
1158.89	1158.86	11	1	11	10	0	10	6.5417		1166.20	1166.18	26	0	26	25	1	25	8.9146	
	1158.89	14	3	11	14	2	12	5.9887		1166.31	1166.35	26	1	25	25	2	24	5.9280	
1159.16	1159.16	18	1	17	18	0	18	3.6090		1166.67	1166.64	15	5	11	15	4	12	4.5809	
1159.32	1159.33	28	4	24	28	3	25	5.3551			1166.69	14	5	9	14	4	10	4.4081	
	1159.34	12	3	9	12	2	10	5.2332			1166.72	27	1	27	26	0	26	8.6456	
1159.48	1159.48	42	5	37	42	4	38	1.7129		1167.00	1166.99	6	5	1	6	4	2	1.4387	
	1159.49	14	0	14	13	1	13	7.9961		1167.20	1167.18	34	3	31	33	4	30	1.5014	
1159.57	1159.57	15	2	14	15	1	15	3.6894			1167.20	28	0	28	27	1	27	8.3422	
1159.68	1159.67	5	2	4	4	1	3	2.0449		1167.33	1167.31	34	6	28	34	5	29	2.5443	
	1159.69	10	3	7	10	2	8	4.4423		1167.43	1167.40	6	4	2	5	3	3	3.3127	
1159.78	1159.77	13	1	13	12	0	12	7.6408		1167.52	1167.51	28	1	27	27	2	26	5.7414	
1160.04	1160.01	32	3	29	32	2	30	3.6337			1167.55	13	3	11	12	2	10	3.1802	
1160.30	1160.27	38	5	33	38	4	34	2.4571		1167.72	1167.72	29	1	29	28	0	28	8.0155	
	1160.32	13	3	11	13	2	12	5.0457			1167.75	37	6	32	37	5	33	1.9922	
1160.46	1160.43	20	1	19	20	0	20	3.1720		1167.95	1167.94	12	3	9	11	2	10	2.9401	
	1160.48	15	3	13	15	2	14	5.2988			1167.98	35	6	30	35	5	31	2.3469	
1160.71	1160.71	16	0	16	15	1	15	8.8276		1168.20	1168.21	30	0	30	29	1	29	7.6665	
	1160.75	18	1	17	17	2	16	4.7414		1168.29	1168.27	15	3	13	14	2	12	3.2105	
1161.03	1161.00	36	5	31	36	4	32	2.8004		1168.38	1168.37	30	6	24	30	5	25	3.2499	
	1161.07	19	3	17	19	2	18	5.1981		1168.52	1168.50	29	2	28	28	1	27	5.6145	
1161.18	1161.16	19	2	18	19	1	19	3.2117		1168.61	1168.61	30	1	29	29</				

TABLE III (Continued)

Line Position (in cm ⁻¹)		Quantum Numbers							Line Position (in cm ⁻¹)		Quantum Numbers								
Exptl.	Theor.	J'	K' ₋₁	K' ₁	J''	K'' ₋₁	K'' ₁	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K' ₋₁	K' ₁	J''	K'' ₋₁	K'' ₁	$\frac{I^o}{C'}$		
		1168.76	28	6	22	28	5	23	3.5837	1176.76	1176.76	18	8	10	18	7	11	3.2214	
		1168.77	29	6	24	29	5	25	3.4167	1177.07	1177.06	12	8	4	12	7	5	2.1942	
1168.98	1169.02	27	6	22	27	5	23	3.7363			1177.10	1177.17	49	1	49	48	0	48	1.8783
1169.22	1169.21	32	0	32	31	1	31	6.9266	1177.20	1177.17	49	1	49	48	0	48	1.5961		
		1169.26	25	6	20	25	5	21	4.0100	1177.32	1177.30	11	6	6	10	5	5	4.2495	
1169.32	1169.33	24	6	18	24	5	19	4.1240	1177.41	1177.38	17	5	13	16	4	12	3.7067		
1169.54	1169.55	22	6	16	22	5	17	4.2921			1177.40	22	4	18	21	3	19	2.5615	
1169.63	1169.66	21	6	16	21	5	17	4.3254	1177.90	1177.90	12	6	6	11	5	7	4.2210		
		1169.67	32	1	31	31	2	30	4.9883	1178.25	1178.28	7	7	1	6	6	0	4.6161	
1169.80	1169.82	19	6	14	19	5	15	4.3617	1178.43	1178.44	36	9	27	36	8	28	1.4496		
1169.94	1169.96	17	6	12	17	5	13	4.2603	1178.60	1178.58	35	9	27	35	8	28	1.5651		
1170.10	1170.08	15	6	10	15	5	11	4.0216	1178.90	1178.89	8	7	1	7	6	2	4.5529		
1170.20	1170.19	13	6	8	13	5	9	3.6306			1178.94	24	4	20	23	3	21	2.1524	
		1170.19	34	0	34	33	1	33	6.1576	1178.99	1178.96	32	9	23	32	8	24	1.9216	
		1170.23	12	6	6	12	5	7	3.3512	1179.46	1179.49	27	9	19	27	8	20	2.4697	
1170.31	1170.27	25	3	23	24	2	22	3.3749			1179.50	9	7	3	8	6	2	4.5036	
		1170.27	11	6	6	11	5	7	3.0034	1179.55	1179.54	21	5	17	20	4	16	3.2311	
		1170.31	10	6	4	10	5	5	2.7237			1179.58	26	9	17	26	8	18	2.5204
		1170.34	33	2	32	32	1	31	4.7563	1179.68	1179.67	25	9	17	25	8	18	2.6054	
1170.65	1170.68	35	1	35	34	0	34	5.7715			1179.68	15	6	10	14	5	9	4.0589	
1171.03	1171.05	12	4	8	11	3	9	3.6027	1179.81	1179.83	23	9	15	23	8	16	2.7489		
1171.19	1171.16	36	0	36	35	1	35	5.3892	1180.05	1180.04	20	9	11	20	8	12	2.7809		
1171.29	1171.28	35	2	34	34	1	33	4.2481	1180.29	1180.26	16	6	10	15	5	11	3.9776		
1171.40	1171.44	7	5	3	6	4	2	3.8878			1180.28	16	9	7	16	8	8	2.4752	
1171.50	1171.53	34	7	27	34	6	28	2.2343			1180.33	15	9	7	15	8	8	2.3212	
1171.60	1171.64	37	1	37	36	0	36	5.0134	1180.69	1180.71	11	7	5	10	6	4	4.4112		
1171.76	1171.77	33	7	27	33	6	28	2.3927	1181.34	1181.32	12	7	5	11	6	6	4.3578		
1171.86	1171.88	33	3	31	32	2	30	3.0935			1181.37	24	5	19	23	4	20	2.7568	
1172.09	1172.05	8	5	3	7	4	4	3.9194	1181.89	1181.91	13	7	7	12	6	6	4.2958		
1172.12	1172.17	38	0	38	37	1	37	4.6462	1181.99	1181.99	19	6	14	18	5	13	3.6572		
1172.22	1172.17	30	7	23	30	6	24	2.8660	1182.26	1182.29	33	10	24	33	9	25	1.5309		
		1172.22	37	2	36	36	1	35	3.7267			1182.30	8	8	0	7	7	1	4.7038
		1172.25	14	4	10	13	3	11	3.5585	1182.40	1182.40	32	10	22	32	9	23	1.6311	
1172.55	1172.51	35	3	33	34	2	32	2.8587	1182.53	1182.51	14	7	7	13	6	8	4.2237		
		1172.55	27	7	21	27	6	22	3.2991			1182.51	31	10	22	31	9	23	1.7294
1172.59	1172.59	39	1	39	38	0	38	4.2906			1182.56	20	6	14	19	5	15	3.5277	
1173.04	1173.04	22	7	15	22	6	16	3.7692	1182.63	1182.61	30	10	20	30	9	21	1.8259		
		1173.06	40	0	40	39	1	39	3.9477	1182.77	1182.77	29	5	25	28	4	24	1.9713	
1173.15	1173.12	21	7	15	21	6	16	3.8155			1182.81	28	10	18	28	9	19	2.0047	
		1173.16	39	2	38	38	1	37	3.2142	1182.93	1182.90	27	10	18	27	9	19	2.0873	
1173.33	1173.34	18	7	11	18	6	12	3.7734			1182.91	9	8	2	8	7	1	4.6166	
1173.53	1173.51	15	7	9	15	6	10	3.4216	1183.05	1183.07	25	10	16	25	9	17	2.2155		
		1173.53	41	1	41	40	0	40	3.6193	1183.18	1183.15	24	10	14	24	9	15	2.2634	
		1173.56	14	7	7	14	6	8	3.2679	1183.50	1183.50	19	10	10	19	9	11	2.2419	
1173.99	1174.00	42	0	42	41	1	41	3.3067			1183.52	10	8	2	9	7	3	4.5394	
1174.18	1174.19	34	8	26	34	7	27	1.9510	1183.70	1183.68	22	6	16	21	5	17	3.2426		
1174.49	1174.47	12	5	7	11	4	8	3.9738			1183.69	16	7	9	15	6	10	4.0463	
		1174.52	19	4	16	18	3	15	3.1785	1184.23	1184.21	23	6	18	22	5	17	3.0900	
1174.73	1174.70	18	4	14	17	3	15	3.2146			1184.27	17	7	11	16	6	10	3.9408	
1175.01	1175.01	43	2	42	42	1	41	2.7294	1184.69	1184.72	12	8	4	11	7	5	4.3880		
1175.18	1175.19	34	8	26	34	7	27	1.9510	1184.78	1184.77	24	6	18	23	5	19	2.9318		
1175.36	1175.33	33	8	26	33	7	27	2.0896	1184.89	1184.85	18	7	11	17	6	12	3.8250		
		1175.38	45	1	45	44	0	44	2.4696	1185.30	1185.32	13	8	6	12	7	5	4.3060	
1175.72	1175.71	30	8	22	30	7	23	2.5023	1185.40	1185.43	19	7	13	18	6	12	3.6993		
1175.90	1175.94	28	8	20	28	7	21	2.7590	1185.87	1185.85	26	6	20	25	5	21	2.6066		
1175.99	1176.00	20	4	16	19	3	17	2.9217	1186.01	1186.00	20	7	13	19	6	14	3.5649		
1176.40	1176.38	27	4	24	26	3	23	2.2570			1186.01	30	11	19	30	10	20	1.5172	
		1176.41	23	8	16	23	7	17	3.2253	1186.14	1186.11	29	11	19	29	10	20	1.5953	
1176.62	1176.63	20	8	12	20	7	13	3.2975	1186.23	1186.20	28	11	17	28	10	18	1.6644		

TABLE III (Continued)

Line Position (in cm^{-1})		Quantum Numbers								Line Position (in cm^{-1})		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\frac{I^o}{n''h'}$	C'	Exptl.	Theor.	J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\frac{I^o}{n''h'}$	C'
1186.53	1186.51	15	8	8	14	7	7	4.1196		1193.35	1193.32	15	10	6	14	9	5	3.8143	
	1186.54	24	11	13	24	10	14	1.8513			1193.33	27	8	20	26	7	19	2.4321	
	1186.57	21	7	15	20	6	14	3.4270			1193.38	22	13	9	22	12	10	1.1629	
1187.23	1187.27	29	6	24	28	5	23	2.1184		1193.61	1193.63	18	13	5	18	12	6	0.9632	
1187.47	1187.52	11	9	3	10	8	2	4.4136		1193.71	1193.73	16	13	3	16	12	4	0.7488	
1187.68	1187.69	17	8	10	16	7	9	3.8988		1193.87	1193.88	28	8	20	27	7	21	2.2700	
1187.97	1187.96	30	6	24	29	5	25	1.9559			1193.89	16	10	6	15	9	7	3.6923	
1188.12	1188.12	12	9	3	11	8	4	4.3169		1194.25	1194.27	11	11	1	10	10	0	4.0346	
1188.24	1188.24	24	7	17	23	6	18	2.9621		1194.46	1194.41	29	8	22	28	7	21	2.1156	
	1188.27	18	8	10	17	7	11	3.7756			1194.48	17	10	8	16	9	7	3.5695	
1188.70	1188.72	13	9	5	12	8	4	4.2182		1194.88	1194.88	12	11	1	11	10	2	3.9127	
1188.95	1188.98	33	6	28	32	5	27	1.5117		1195.06	1195.06	18	10	8	17	9	9	3.4404	
1189.26	1189.29	31	12	20	31	11	21	1.1782			1195.10	24	9	15	23	8	16	2.7745	
1189.36	1189.32	14	9	5	13	8	6	4.1153		1195.43	1195.47	31	8	24	30	7	23	1.8284	
	1189.39	30	12	18	30	11	19	1.2443			1195.48	13	11	3	12	10	2	3.7940	
1189.52	1189.48	29	12	18	29	11	19	1.3025		1195.64	1195.64	19	10	10	18	9	9	3.3070	
	1189.57	28	12	16	28	11	17	1.3560			1195.66	25	9	17	24	8	16	2.6211	
1189.73	1189.74	26	12	14	26	11	15	1.4432		1195.99	1195.99	32	8	24	31	7	25	1.6755	
1189.83	1189.82	25	12	14	25	11	15	1.4742		1196.22	1196.21	26	9	17	25	8	18	2.4751	
	1189.87	27	7	21	26	6	20	2.4777			1196.22	20	10	10	19	9	11	3.1695	
1189.93	1189.90	24	12	12	24	11	13	1.4923		1196.47	1196.50	33	8	26	32	7	25	1.5390	
	1189.91	15	9	7	14	8	6	4.0068		1196.64	1196.67	15	11	5	14	10	4	3.5567	
1190.02	1189.99	21	8	14	20	7	13	3.3620		1196.98	1197.01	34	8	26	33	7	27	1.4083	
	1190.04	22	12	10	22	11	11	1.4991		1197.24	1197.26	16	11	5	15	10	6	3.4352	
1190.17	1190.17	20	12	8	20	11	9	1.4424		1197.34	1197.31	28	9	19	27	8	20	2.16'9	
1190.44	1190.41	28	7	21	27	6	22	2.3167			1197.37	22	10	12	21	9	13	2.8856	
1190.58	1190.56	22	8	14	21	7	15	3.2155		1197.81	1197.85	17	11	7	16	10	6	3.3110	
1191.05	1191.09	17	9	9	16	8	8	3.7706			1197.85	29	9	21	28	8	20	2.0291	
1192.07	1192.11	13	10	4	12	9	3	4.0434		1197.93	1197.93	23	10	14	22	9	13	2.7406	
1192.26	1192.24	25	8	18	24	7	17	2.7441		1198.06	1198.02	36	8	28	35	7	29	1.1663	
	1192.25	19	9	11	18	8	10	3.5088		1198.26	1198.23	12	12	0	11	11	1	3.6096	
1192.73	1192.70	14	10	4	13	9	5	3.9303		1198.42	1198.39	30	9	21	29	8	22	1.8731	
1192.83	1192.79	26	8	18	25	7	19	2.5853			1198.44	18	11	7	17	10	8	3.1838	
	1192.83	20	9	11	19	8	12	3.3694		1198.90	1198.92	31	9	23	30	8	22	1.7333	
1192.99	1193.01	27	13	15	27	12	16	1.1176		1199.45	1199.43	14	12	2	13	11	3	3.3690	
1193.09	1193.09	26	13	13	26	12	14	1.1452			1199.45	32	9	23	31	8	24	1.5983	
1193.20	1193.17	25	13	13	25	12	14	1.1649		1199.58	1199.60	20	11	9	19	10	10	2.9216	
	1193.24	24	13	11	24	12	12	1.1753			1199.63	26	10	16	25	9	17	2.2873	

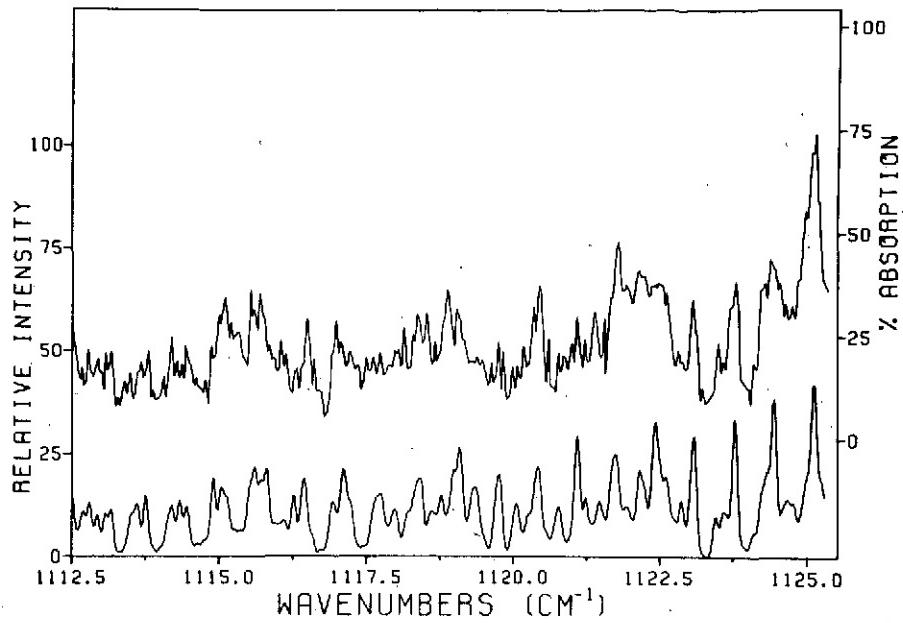


Fig. 1(a). Experimental and theoretical spectra of v_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1112.5 to 1125.0 cm^{-1} .

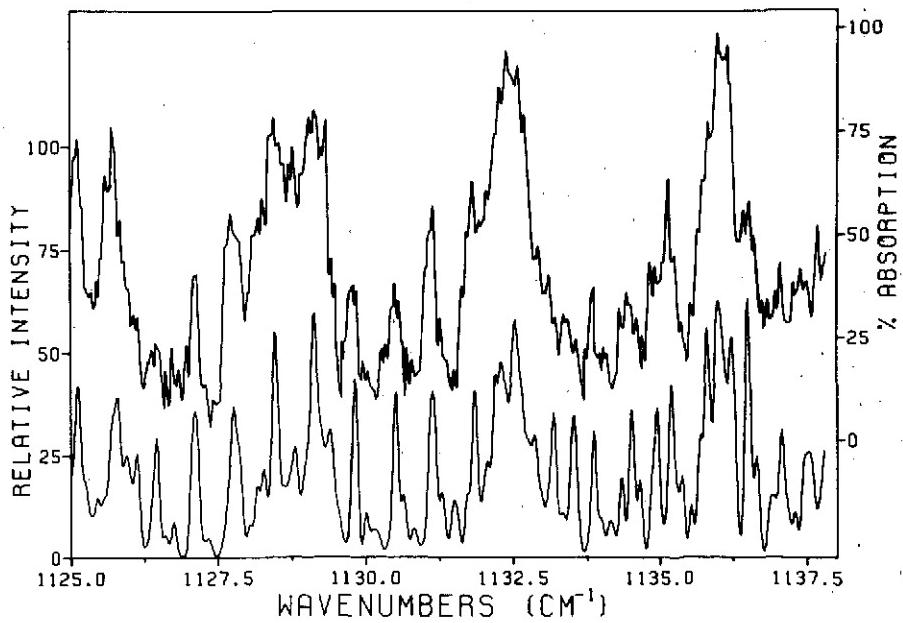


Fig. 1(b). Experimental and theoretical spectra of v_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1125.0 to 1137.5 cm^{-1} .

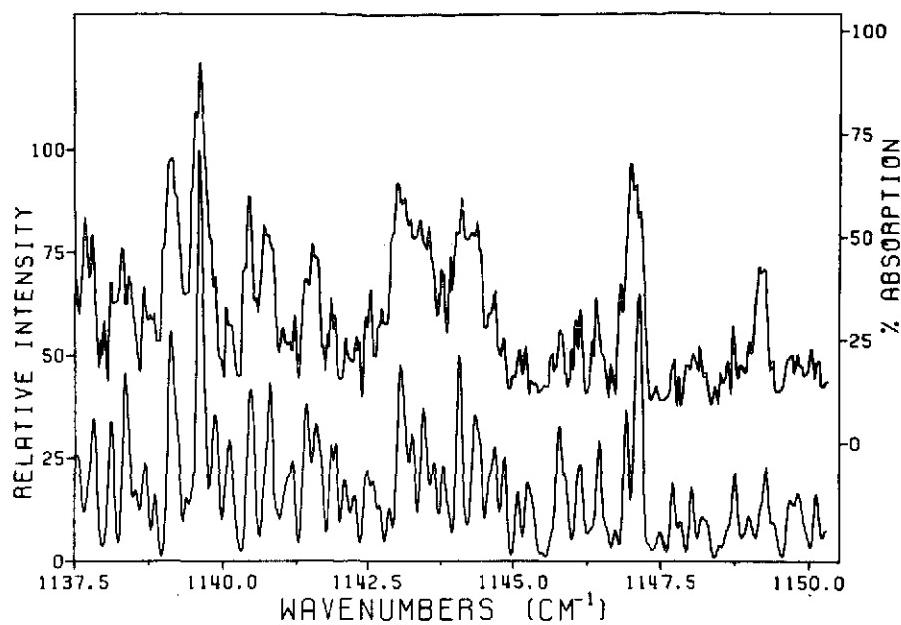


Fig. 1(c). Experimental and theoretical spectra of ν_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1137.5 to 1150.0 cm^{-1} .

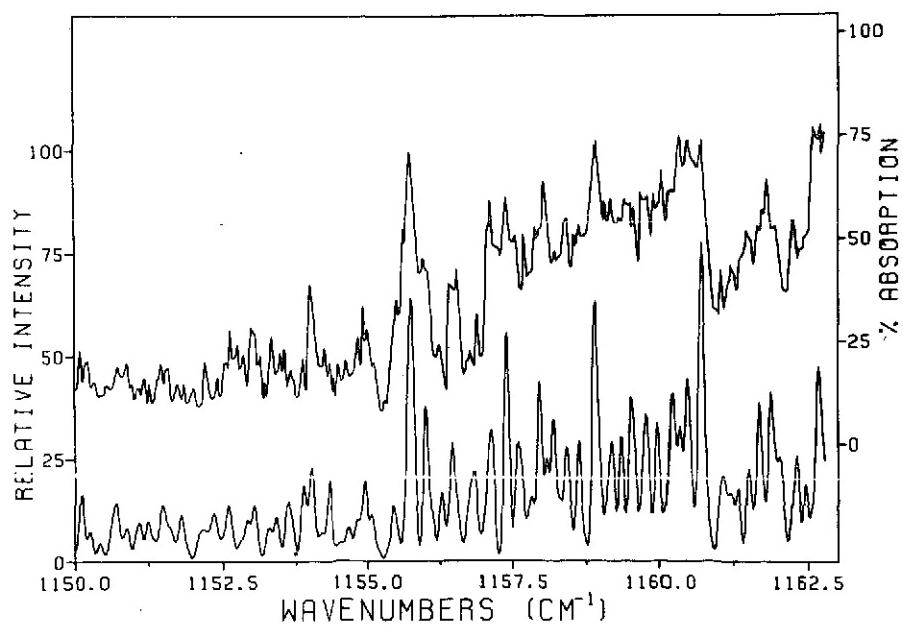


Fig. 1(d). Experimental and theoretical spectra of ν_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1150.0 to 1162.5 cm^{-1} .

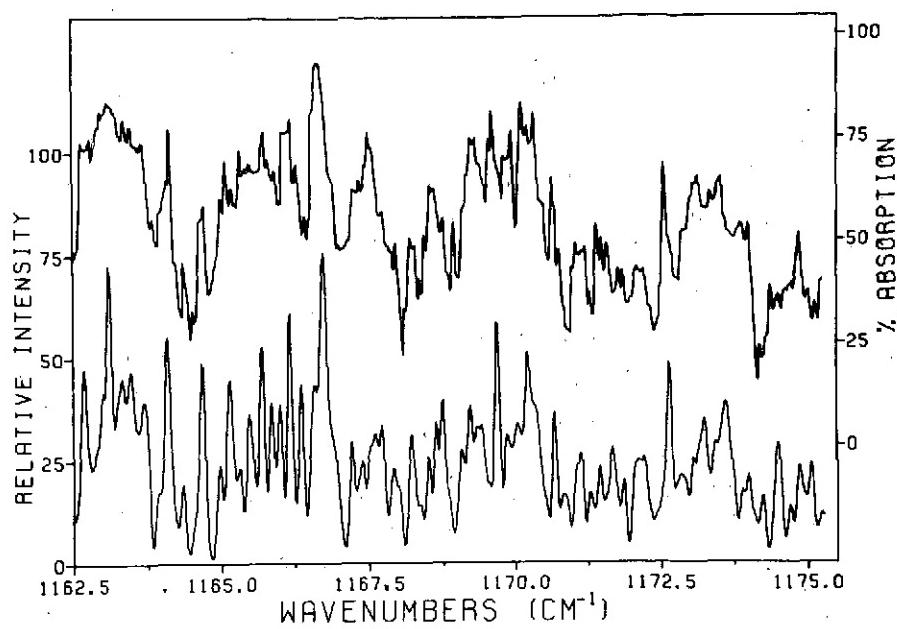


Fig. 1(e). Experimental and theoretical spectra of ν_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1162.5 to 1175.0 cm^{-1} .

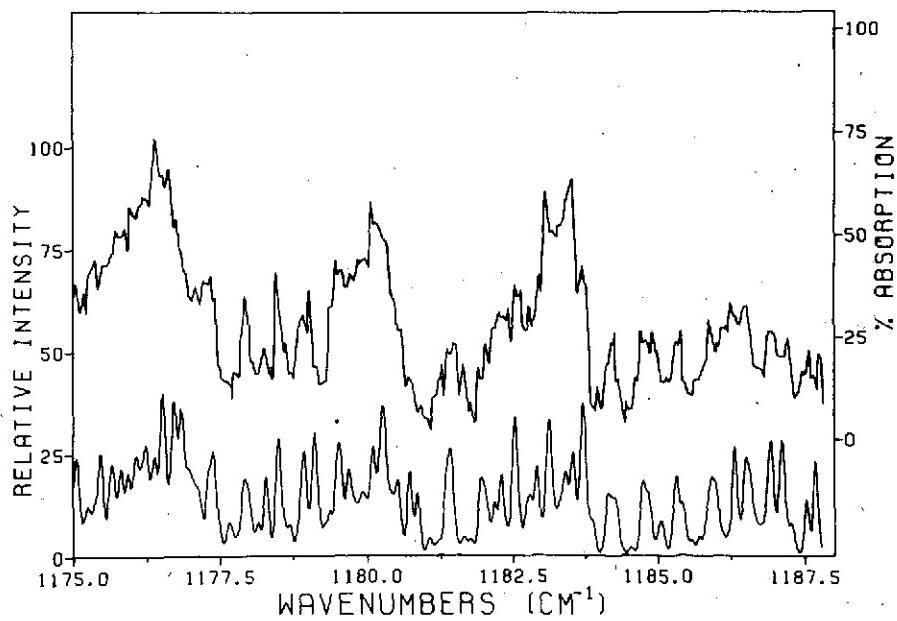


Fig. 1(f). Experimental and theoretical spectra of ν_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1175.0 to 1187.5 cm^{-1} .

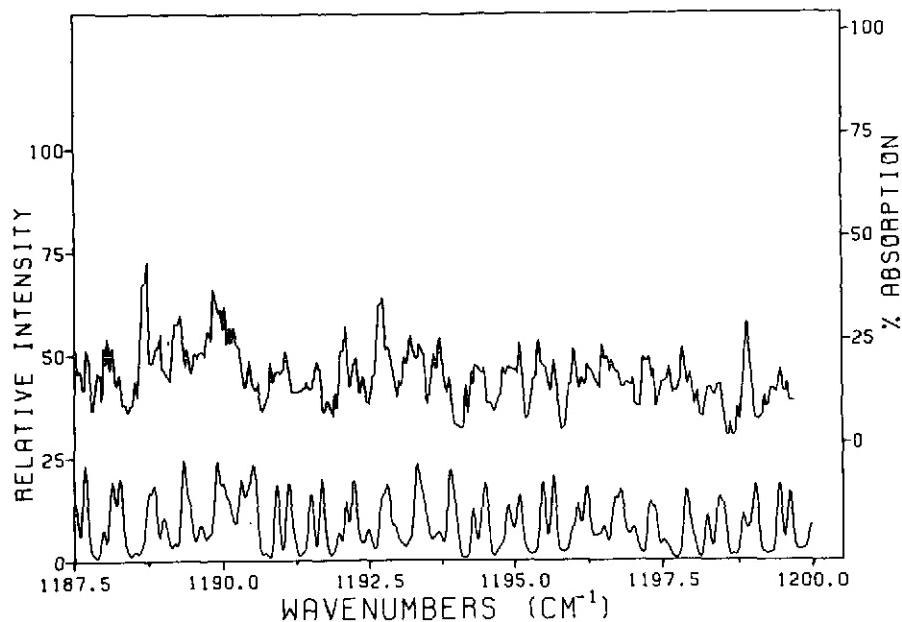


Fig. 1(g). Experimental and theoretical spectra of v_1 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1187.5 to 1200.0 cm^{-1} .

lines in Table I of Ref. 8, and have determined that the two sets of values agree to 0.01 cm^{-1} except for a single line with $J = 30$ for which the apparent discrepancy is only 0.02 cm^{-1} . Subsequently, from a more extensive tabulation provided by Hinkley [Appendix B of Ref. 30] we found that for all lines with $J \leq 46$, of which there are 78, the maximum difference in the calculated line positions was 0.02 cm^{-1} . These differences may be attributed to the small disparities in assumed excited-state centrifugal distortion constants.

In Fig. 2 and Table IV, we have compared our experimental and theoretical results for v_2 in the spectral range from 470 to 590 cm^{-1} . The selection rules for this band²⁵ are the same as those for v_1 , described above. Because of the lower resolution available in the v_2 region, we have been able to assign only approximately 180 observed lines. Strong well-defined peaks in Fig. 2 correspond to Q sub-branches. A sub-branch, in the case of a nearly prolate symmetric top, is characterized by a constant value of K_{-1} and the parity of the initial state. Individual lines in these sub-branches are in most cases unresolved. In Table IV, the subscripts to Q denote the changes in K_{-1} and K_1 . The initial state of the transitions is given in parentheses. For low values of K_{-1} , the even- and odd-parity

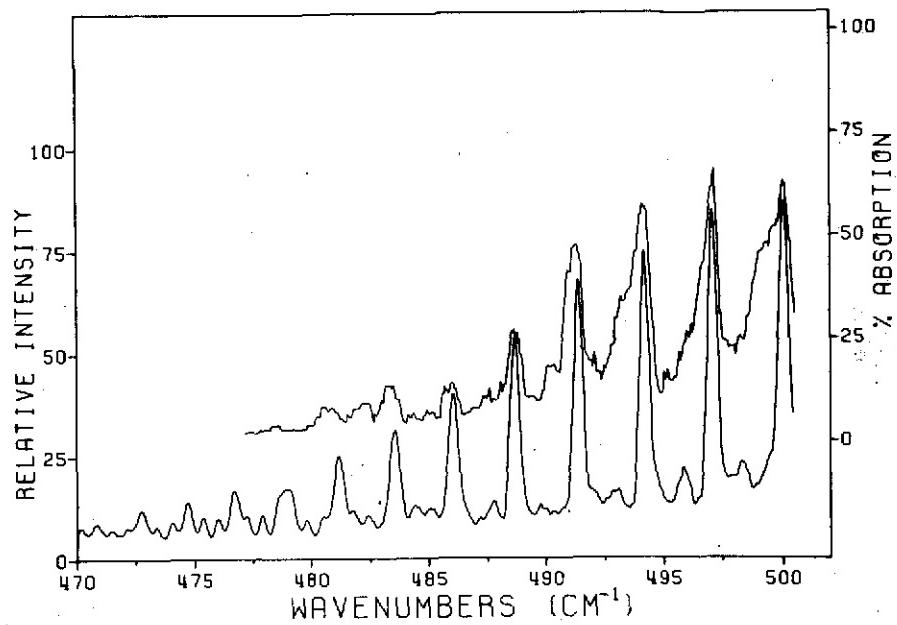


Fig. 2(a). Experimental and theoretical spectra of v_2 band of $^{32}\text{S}^{16}\text{O}_2$ in range 470 to 500 cm^{-1} .

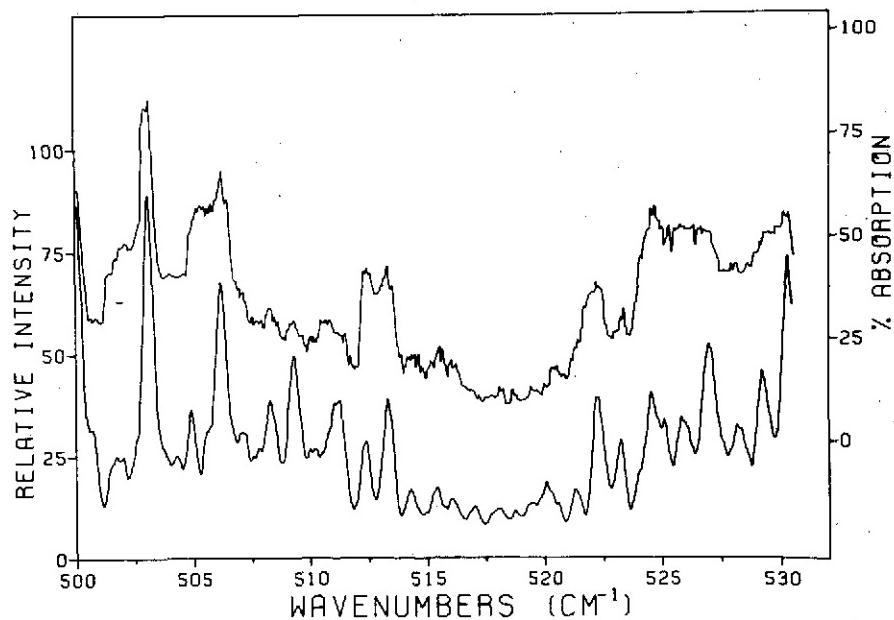


Fig. 2(b). Experimental and theoretical spectra of v_2 band of $^{32}\text{S}^{16}\text{O}_2$ in range 500 to 530 cm^{-1} .

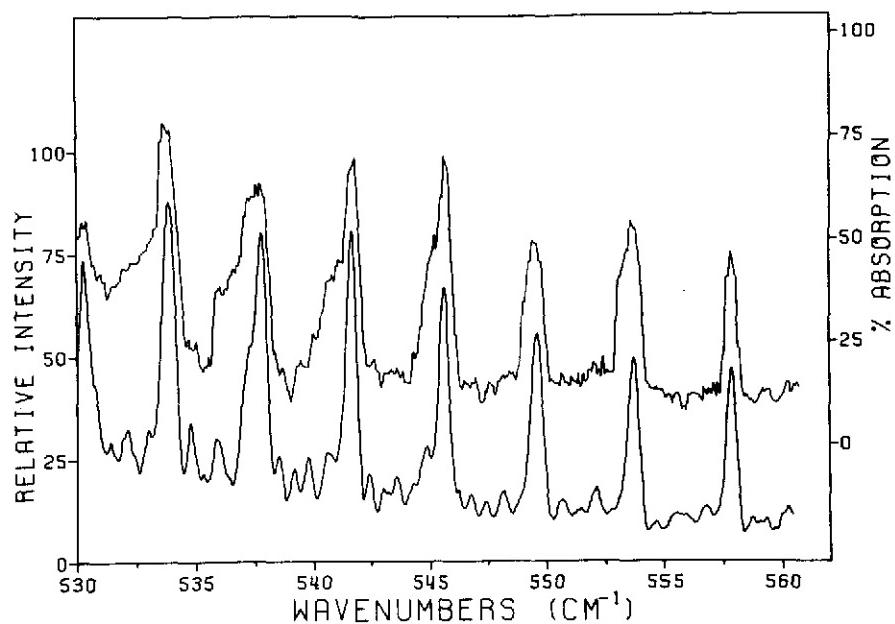


Fig. 2(c). Experimental and theoretical spectra of ν_2 band of $^{32}\text{S}^{16}\text{O}_2$ in range 530 to 560 cm^{-1} .

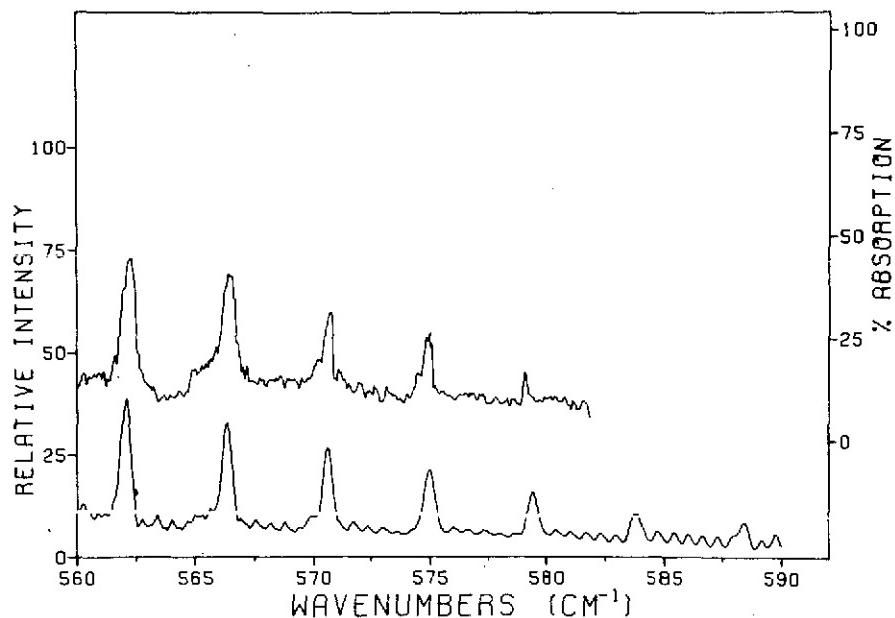


Fig. 2(d). Experimental and theoretical spectra of ν_2 band of $^{32}\text{S}^{16}\text{O}_2$ in range 560 to 590 cm^{-1} .

TABLE IV

COMPARISON OF EXPERIMENTAL AND THEORETICAL SPECTRAL LINE POSITIONS, WITH QUANTUM NUMBER ASSIGNMENTS, FOR THE v_2 BAND OF $^{32}\text{S}^{16}\text{O}_2$ CENTERED AT $517.75 \pm 0.10 \text{ cm}^{-1}$. LINE INTENSITIES [SEE SEC. III, ESPECIALLY EQ.(6)] ARE COMPUTED AT 300°K. SEE SEC. III FOR Q SUB-BRANCH NOTATION.

Line Position		Quantum Numbers								Line Position		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$		
477.85	477.87	12	10	2	13	11	3	2.4590	496.19	496.17	5	5	1	6	6	0	3.3267		
	477.93	20	8	12	21	9	13	2.1097	497.14	$Q_{11}^-(J, 7, K_1)$ sub-branch									
478.56	478.51	11	10	2	12	11	1	2.5494	498.28	498.25	24	2	22	25	3	23	2.6347		
	478.58	19	8	12	20	9	11	2.2158		498.31	31	1	31	32	0	32	5.4562		
480.48	480.44	12	9	3	13	10	4	2.6890	499.31	499.36	29	2	28	30	1	29	4.2949		
	480.52	16	8	8	17	9	9	2.5200	499.98	$Q_{11}^-(J, 6, K_1)$ sub-branch									
480.85	480.86	29	5	25	30	6	24	1.3175	500.62	500.64	26	1	25	27	2	26	4.7135		
	481.05	$Q_{11}^-(J, 13, K_1)$ sub-branch								500.66	27	2	26	28	1	27	4.6028		
481.60	481.66	23	6	18	24	7	17	2.0091	500.81	500.77	27	1	27	28	0	28	6.6981		
482.68	482.65	56	0	56	57	1	57	0.3980		500.82	41	4	38	41	5	37	1.1296		
482.93	482.85	26	5	21	27	6	22	1.6756	501.67	501.64	24	1	23	25	2	24	4.8564		
	482.93	21	6	16	22	7	15	2.2448		501.72	12	2	10	13	3	11	2.5632		
483.38	$Q_{11}^-(J, 12, K_1)$ sub-branch								501.87	501.88	34	1	33	34	2	32	1.5773		
484.16	484.21	19	6	14	20	7	13	2.4710	502.08	501.99	25	1	25	26	0	26	7.2273		
484.39	484.39	10	8	2	11	9	3	3.0456		502.08	38	5	33	38	6	32	1.5618		
484.90	484.86	18	6	12	19	7	13	2.5782	503.13	$Q_{11}^-(J, 5, K_1)$ sub-branch									
	484.93	27	4	24	28	5	23	1.4360		505.32	505.41	25	3	23	25	4	22	3.9681	
485.25	485.22	13	7	7	14	8	6	2.9402	505.48	505.44	32	4	28	32	5	27	2.9251		
	485.30	22	5	17	23	6	18	2.1642		505.52	5	2	4	6	3	3	2.2454		
485.67	485.68	8	8	0	9	9	1	3.2192		505.56	14	1	13	15	2	14	3.6774		
485.96	$Q_{11}^-(J, 11, K_1)$ sub-branch								505.85	505.89	21	3	19	21	4	18	4.4600		
487.65	487.68	23	4	20	24	5	19	1.9687	506.20	$Q_{11}^-(J, 4, K_1)$ sub-branch									
	487.73	48	0	48	49	1	49	1.1589	506.53	506.48	16	3	13	16	4	12	4.4691		
488.04	488.07	13	6	8	14	7	7	3.0237		506.53	19	2	18	20	1	19	4.4779		
	488.65	$Q_{11}^-(J, 10, K_1)$ sub-branch								506.57	23	2	22	23	3	21	3.7980		
490.03	490.01	10	6	4	11	7	5	3.2090		506.60	7	1	7	8	2	6	1.4297		
	490.07	44	1	43	45	2	44	1.3835	506.99	506.95	17	1	17	18	0	18	7.8932		
490.32	490.25	19	4	16	20	5	15	2.4576		507.01	10	1	9	11	2	10	2.8783		
	490.39	14	5	9	15	6	10	2.9680	507.17	507.21	16	0	16	17	1	17	7.7478		
490.90	490.87	43	1	43	44	0	44	2.0315	507.53	507.46	2	2	0	3	3	1	2.0263		
	490.91	42	2	40	43	3	41	1.2273		507.57	22	3	19	22	4	18	4.8466		
	490.95	18	4	14	19	5	15	2.5685	508.26	$Q_{11}^-(J, 3, K_1)$ sub-branch									
491.30	$Q_{11}^-(J, 9, K_1)$ sub-branch								508.45	508.45	21	3	19	22	2	20	2.2442		
492.02	492.04	40	2	38	41	3	39	1.4625	508.64	508.60	26	3	23	26	4	22	4.8183		
	492.12	41	1	41	42	0	42	2.4830		508.67	15	2	14	15	3	13	4.5439		
492.46	492.51	40	1	39	41	2	40	2.0497	509.30	$eQ_{11}^-(J, 3, K_1)$ sub-branch									
492.70	492.74	40	0	40	41	1	41	2.7311		510.03	509.97	12	2	10	12	3	9	4.5384	
492.92	492.95	10	5	5	11	6	6	3.1747		510.03	28	2	26	28	3	25	4.8929		
493.13	493.06	19	3	17	20	4	16	2.1821		510.06	25	4	22	26	3	23	1.3605		
	493.12	38	2	36	39	3	37	1.7086	510.20	510.21	13	1	13	13	2	12	3.2827		
	493.15	39	2	38	40	1	39	2.2403		510.52	510.52	22	1	21	22	2	20	5.2404	
494.15	$Q_{11}^-(J, 8, K_1)$ sub-branch									510.54	19	3	17	20	2	18	2.0789		
495.04	495.09	34	2	32	35	3	33	2.1816		510.72	510.70	16	2	14	16	3	13	5.8705	
495.24	495.23	36	0	36	37	1	37	3.8556		510.89	510.89	11	1	11	11	2	10	3.2481	
495.65	495.61	35	2	34	36	1	35	3.0684		510.96	11	1	11	12	0	12	6.0013		
495.95	495.85	35	1	35	36	0	36	4.1650		511.57	511.59	20	1	19	20	2	18	6.1756	
	495.93	32	2	30	33	3	31	2.3743		511.75	511.77	13	2	12	14	1	13	2.9435	

TABLE IV (Continued)

Line Position (in cm ⁻¹)		Quantum Numbers								Line Position (in cm ⁻¹)		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_{1}	J''	K''_{-1}	K''_{1}	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K'_{-1}	K'_{1}	J''	K''_{-1}	K''_{1}	$\frac{I^o}{C'}$		
512.28	512.23	6	0	6	7	1	7	3.6483	\$26.95	${}^0Q_{11}^-$	(J, 2, K ₁)	sub-branch							
	512.24	14	0	14	14	1	13	4.1510	527.71	527.72	26	2	24	26	1	25	3.8469		
512.47		${}^0Q_{11}^-$	(J, 2, K ₁)	sub-branch					527.92	527.85	9	2	8	8	1	7	2.7471		
512.62	512.60	17	3	15	18	2	16	1.9041		527.89	19	2	18	19	1	19	2.9963		
513.30		${}^eQ_{11}^-$	(J, 2, K ₁)	sub-branch						527.96	32	3	29	32	2	30	3.3811		
513.53	513.46	10	1	9	10	2	8	5.7682	528.16	528.13	17	1	17	16	0	16	8.5646		
	513.49	12	1	11	12	2	10	6.8287	528.63	528.65	11	2	10	10	1	9	3.1947		
513.57	11	2	10	12	1	11	2.3714		528.69	22	4	18	22	3	19	5.2661			
513.93	513.87	7	1	7	8	0	8	3.7376	528.90	528.90	13	6	8	14	5	9	0.7189		
	513.93	17	4	14	16	5	11	1.0946	529.12	529.05	20	1	19	19	2	18	4.9613		
514.13	514.12	22	5	17	21	6	16	1.0021	529.25	${}^eQ_{11}^-$	(J, 3, K ₁)	sub-branch							
514.29	514.25	10	0	10	10	1	9	5.0873	529.65	529.59	18	4	14	18	3	15	5.1451		
	514.32	21	4	18	22	3	19	1.4202	529.80	529.82	36	5	31	36	4	32	2.6035		
514.52	514.47	13	3	11	12	4	8	1.0624	530.07	530.07	14	4	10	14	3	11	4.6422		
	514.58	15	3	13	16	2	14	1.7210	530.24	${}^oQ_{11}^-$	(J, 3, K ₁)	sub-branch							
514.67	514.64	18	4	14	17	5	13	1.1410	530.70	530.73	17	2	16	16	1	15	4.6239		
514.90	514.94	8	0	8	8	1	7	5.1415		530.74	22	0	22	21	1	21	8.9777		
515.17	515.22	24	4	20	25	3	23	1.0300	530.90	530.86	42	4	38	42	3	39	1.3252		
	515.24	19	4	16	18	5	13	1.1729		530.92	36	3	33	36	2	34	2.0955		
515.48	515.44	6	0	6	6	1	5	4.6843	533.31	533.28	11	3	9	10	2	8	2.9320		
515.68	515.67	29	6	24	28	7	21	0.7352		533.29	24	5	19	24	4	20	4.3585		
	515.74	15	3	13	14	4	10	1.2221	533.64	533.63	27	1	27	26	0	26	8.1316		
516.03	516.02	20	4	16	19	5	15	1.1980		533.64	30	1	29	30	0	30	1.4294		
	516.04	22	4	18	23	3	21	1.1940	533.93	${}^oQ_{11}^-$	(J, 4, K ₁)	sub-branch							
516.26	516.24	19	4	16	20	3	17	1.4281	534.75	534.75	29	1	29	28	0	28	7.5521		
517.24	517.19	13	2	12	12	3	9	1.2161		534.81	27	2	26	26	1	25	5.5536		
518.12	518.09	15	2	14	14	3	11	1.2397	535.01	535.02	15	3	13	14	2	12	3.0268		
	518.17	18	4	14	19	3	17	1.3614		535.06	39	5	35	39	4	36	1.6190		
518.27	518.23	11	3	9	12	2	10	1.3047	535.43	535.41	8	4	4	7	3	5	3.2619		
518.61	518.63	8	1	7	7	2	6	1.3067	536.00	536.00	30	1	29	29	2	28	5.1082		
518.75	518.72	4	0	4	3	1	3	1.4870		536.60	536.64	35	2	34	35	1	35	0.8993	
	518.75	12	3	9	13	2	12	1.2369	537.20	537.16	23	3	21	22	2	20	3.1552		
518.80	518.80	17	2	16	16	3	13	1.1521		537.20	32	1	31	31	2	30	4.7154		
	519.41	519.43	21	5	17	22	4	18	1.2345		537.26	5	5	1	4	4	0	3.6540	
520.05	520.09	6	1	5	6	0	6	4.7789	${}^oQ_{11}^-$	(J, 5, K ₁)	sub-branch								
520.30	520.33	10	1	9	9	2	8	1.8594	537.77	${}^oQ_{11}^-$	(J, 6, K ₁)	sub-branch							
520.53	520.58	8	1	7	8	0	8	5.2617	538.35	538.37	34	1	33	33	2	32	4.2627		
520.85	520.91	19	5	15	20	4	16	1.2371		538.65	538.63	36	0	36	35	1	35	5.1066	
521.10	521.11	13	4	10	14	3	11	1.1980	539.89	539.80	9	5	5	8	4	4	3.7478		
521.27	521.26	10	1	9	10	0	10	5.2304		539.88	36	2	34	35	3	33	5.5561		
521.68	521.71	18	5	13	19	4	16	1.2200	540.74	540.75	17	4	14	16	3	13	3.2149		
522.25	${}^eQ_{11}^-$	(J, 1, K ₁)	sub-branch						541.05	541.07	11	5	7	10	4	6	3.7836		
523.20	523.20	18	2	16	18	1	17	7.2577		${}^oQ_{11}^-$	(J, 6, K ₁)	sub-branch							
523.37		${}^oQ_{11}^-$	(J, 1, K ₁)	sub-branch						542.60	542.54	21	4	18	20	3	17	2.8059	
524.12	524.18	9	2	8	9	1	9	3.2284		543.02	543.00	8	6	2	7	5	3	4.0887	
524.50		${}^eQ_{11}^-$	(J, 2, K ₁)	sub-branch						543.28	543.21	23	4	20	22	3	19	2.5741	
524.68	524.66	24	3	21	24	2	22	6.7275		543.25	20	4	16	19	3	17	2.7931		
	524.73	11	2	10	11	1	11	3.4597	543.60	543.57	15	5	11	14	4	10	3.6865		
525.00	525.07	26	3	23	26	2	24	6.0346		543.63	9	6	4	8	5	3	4.0833		
525.28	525.33	20	2	18	19	3	17	2.2149	544.24	544.20	16	5	11	15	4	12	3.6229		
525.76	525.77	28	3	25	28	2	26	5.1517		544.26	10	6	4	9	5	5	4.0765		
525.90	525.84	14	0	14	13	1	13	7.4305	${}^oQ_{11}^-$	(J, 7, K ₁)	sub-branch								
526.32	526.32	24	2	22	24	1	23	4.6253	546.43	546.44	24	4	20	23	3	21	2.0716		
526.65	526.67	7	3	5	7	2	6	2.8812		546.91	546.89	8	7	1	7	6	2	4.3657	
	526.72	9	3	7	9	2	8	3.6547	547.48	547.42	15	6	10	14	5	9	3.8951		

TABLE IV (Continued)

Line Position (in cm^{-1})		Quantum Numbers								Line Position (in cm^{-1})		Quantum Numbers							
Exptl.	Theor.	J'	K'\$_{-1}\$	K'\$_1\$	J''	K''\$_{-1}\$	K''\$_1\$	$\frac{I^o}{C'}$	Exptl.	Theor.	J''	K'\$_{-1}\$	K'\$_1\$	J''	K''\$_{-1}\$	K''\$_1\$	$\frac{I^o}{C'}$		
548.09	548.52	9	7	3	8	6	2	4.3220	564.25	564.35	23	9	15	22	8	14	2.8768		
	548.05	16	6	10	15	5	11	3.8209	564.97	564.97	24	9	15	23	8	16	2.7291		
	548.16	10	7	3	9	6	4	4.2826	565.00	565.00	11	11	1	10	10	0	3.9697		
549.47	Q_{11}^- (J, 8, K\$_1\$) sub-branch								565.25	565.23	31	8	24	30	7	23	1.7898		
550.23	550.20	27	5	23	26	4	22	2.2072	565.29	565.29	18	10	8	17	9	9	3.3855		
550.64	550.69	14	7	7	13	6	8	4.0719	565.60	565.60	25	9	17	24	8	16	2.5807		
551.27	551.32	15	7	9	14	6	8	3.9951	565.64	565.64	12	11	1	11	10	2	3.8531		
551.52	551.48	9	8	2	8	7	1	4.4556	565.84	565.84	32	8	24	31	7	25	1.6517		
	551.52	31	5	27	30	4	26	1.6228	565.87	565.87	19	10	10	18	9	9	3.2567		
551.79	551.77	22	6	16	21	5	17	3.1327	566.25	Q_{11}^- (J, 12, K\$_1\$) sub-branch									
	551.84	28	5	23	27	4	24	1.9979	567.15	567.19	21	10	12	20	9	11	2.9881		
552.01	551.95	16	7	9	15	6	10	3.9079	567.67	567.64	35	8	28	34	7	27	1.2692		
552.21	552.23	37	5	33	36	4	32	0.9895	567.82	567.81	22	10	12	21	9	13	2.8494		
552.40	552.37	23	6	18	22	5	17	2.9881	568.40	568.44	23	10	14	22	9	13	2.7087		
553.65	Q_{11}^- (J, 9, K\$_1\$) sub-branch								568.88	568.81	17	11	7	16	10	6	3.2741		
554.66	554.65	14	8	6	13	7	7	4.0882	569.15	569.07	24	10	14	23	9	15	2.5665		
	554.73	27	6	22	26	5	21	2.3718	569.44	569.44	18	11	7	17	10	8	3.1512		
554.97	554.91	32	5	27	31	4	28	1.3379	569.71	569.70	25	10	16	24	9	15	2.4242		
555.25	555.29	15	8	8	14	7	7	3.9971	570.09	570.07	19	11	9	18	10	8	3.0250		
555.55	555.51	9	9	1	8	8	0	4.4820	570.60	Q_{11}^- (J, 13, K\$_1\$) sub-branch									
555.93	555.92	16	8	8	15	7	9	3.8979	571.06	571.11	14	12	2	13	11	3	3.3428		
556.61	556.55	17	8	10	16	7	9	3.7900	571.29	571.34	21	11	11	20	10	10	2.7653		
	556.62	30	6	24	29	5	25	1.9049	571.52	571.57	28	10	18	27	9	19	2.0028		
556.98	556.94	24	7	17	23	6	18	2.8826	571.95	571.97	22	11	11	21	10	12	2.6327		
557.23	557.18	18	8	10	17	7	11	3.6733	572.40	572.38	16	12	4	15	11	5	3.1119		
557.85	Q_{11}^- (J, 10, K\$_1\$) sub-branch								572.62	572.60	23	11	13	22	10	12	2.4991		
558.45	558.43	20	8	12	19	7	13	3.4175	573.08	573.01	17	12	6	16	11	5	2.9948		
558.66	558.68	14	9	5	13	8	6	4.0122	573.45	573.43	31	10	22	30	9	21	1.6058		
559.12	559.06	21	8	14	20	7	13	3.2799	573.70	573.65	18	12	6	17	11	7	2.8760		
	559.09	34	6	28	33	5	29	1.3324	574.01	574.05	32	10	22	31	9	23	1.4819		
559.37	559.31	15	9	7	14	8	6	3.9049	574.48	574.48	26	11	15	25	10	16	2.0981		
	559.38	28	7	21	27	6	22	2.2628	574.95	Q_{11}^- (J, 14, K\$_1\$) sub-branch									
560.20	560.23	10	10	0	9	9	1	4.2829	575.25	575.28	34	10	24	33	9	25	1.2490		
560.43	560.40	36	6	30	35	5	31	1.0795	575.57	575.54	21	12	10	20	11	9	2.5098		
560.65	560.57	17	9	9	16	8	8	3.6857	576.55	576.51	36	10	26	35	9	27	1.0385		
	560.59	30	7	23	29	6	24	1.9594	576.84	576.80	23	12	12	22	11	11	2.2611		
560.87	560.86	11	10	2	10	9	1	4.1726	577.23	577.27	17	13	5	16	12	4	2.6866		
	560.93	24	8	16	23	7	17	2.8393	578.54	578.54	19	13	7	18	12	6	2.4617		
561.15	561.17	31	7	25	30	6	24	1.8125	579.15	Q_{11}^- (J, 15, K\$_1\$) sub-branch									
561.60	561.55	25	8	18	24	7	17	2.6872	580.34	580.31	15	14	2	14	13	1	2.5724		
562.05	Q_{11}^- (J, 11, K\$_1\$) sub-branch									580.43	580.43	22	13	9	21	12	10	2.1207	
563.13	563.09	21	9	13	20	8	12	3.1644	581.05	581.07	23	13	11	22	12	10	2.0073		
563.68	563.72	22	9	13	21	8	14	3.0219	581.55	581.58	17	14	4	16	13	3	2.3647		

sub-branches (corresponding to even- and odd-J transitions, resp., for $^{32}\text{S}^{16}\text{O}_2$) form two separate peaks in a Q sub-branch. As an example, the observed line positions in Table IV at 508.26 and 509.30 cm^{-1} correspond to the ${}^0\text{Q}_{\frac{1}{1}}(\text{J},3,\text{K}_1)$ sub-branch and its even-J analog, resp. The left superscripts denote odd and even parity, resp., of the initial states; and the selection rules are explicitly $\Delta J = 0$, $\Delta K_{-1} = -1$ ($K_{-1} = 3 + 2$ in this example), and $\Delta K_1 = +1$. In the particular cases of ${}^0\text{Q}_{\frac{1}{1}}(\text{J},1,\text{K}_1)$ and ${}^0\text{Q}_{\frac{1}{1}}(\text{J},0,\text{K}_1)$, both of which have only even sub-branches, it has been possible to resolve several individual transitions.

The observed positions of the Q sub-branches in the present work agree with those given previously by Shelton *et al.*¹ We have determined the band center of v_2 to be at $517.75 \pm 0.10 \text{ cm}^{-1}$. This value may be compared with the earlier results: 524 (Ref. 26), 517.84 (Ref. 27), 517.69 (Ref. 1), and $518.0 \pm 0.5 \text{ cm}^{-1}$ (Ref. 28).

The experimental and theoretical results for v_3 in the spectral range from 1327.5 to 1390.0 cm^{-1} are represented in Fig. 3 and Table V. The selection rules,²⁵ different from those for v_1 and v_2 , are $\Delta J = 0, \pm 1$; $J = 0 \leftrightarrow J = 0$; but $\Delta K_{-1} = 0, \pm 2, \dots$; and $\Delta K_1 = \pm 1, \pm 3, \dots$. Because of the relatively large number of strong, closely spaced lines in v_3 ,

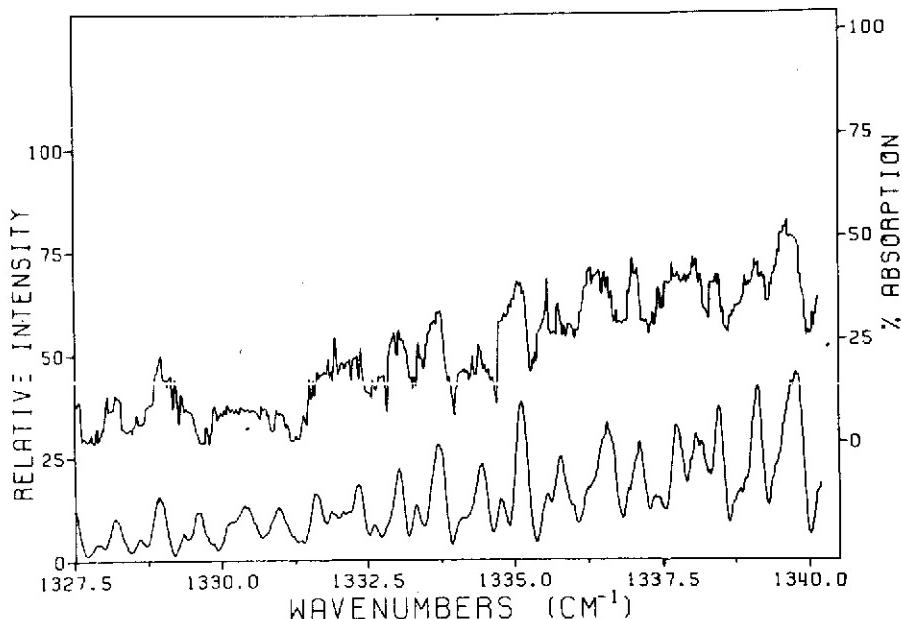


Fig. 3(a). Experimental and theoretical spectra of v_3 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1327.5 to 1340.0 cm^{-1} .

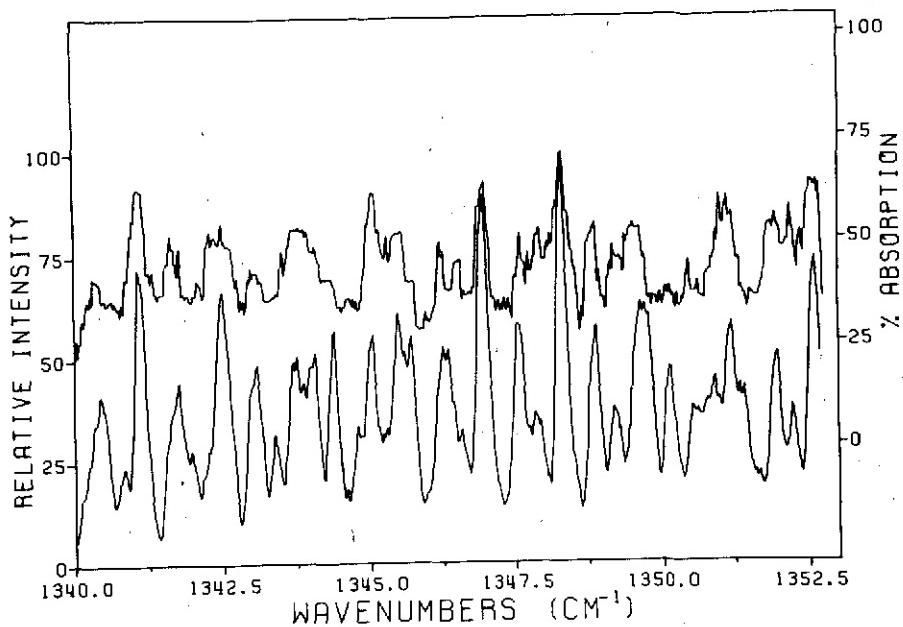


Fig. 3(b). Experimental and theoretical spectra of v_3 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1340.0 to 1352.5 cm^{-1} .

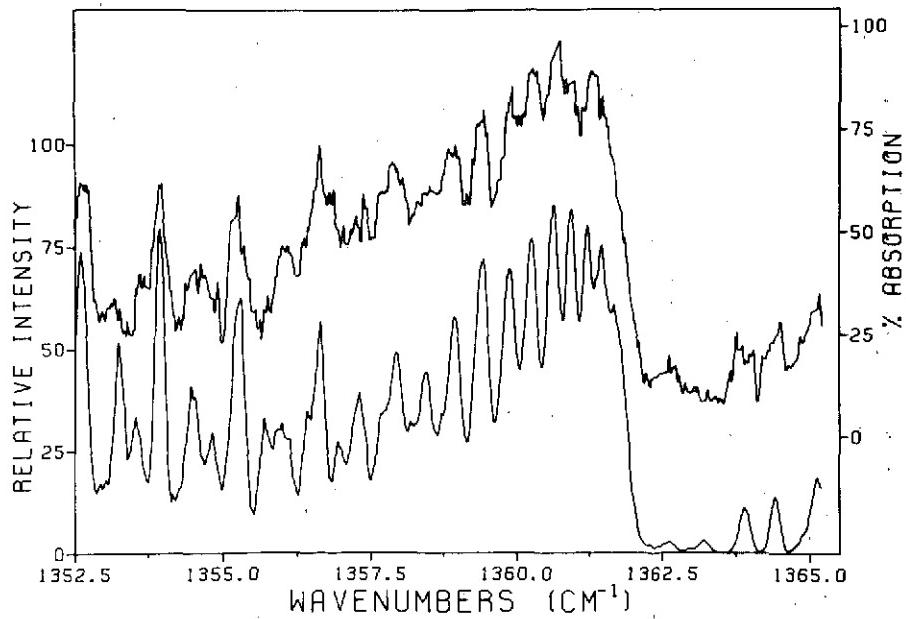


Fig. 3(c). Experimental and theoretical spectra of v_3 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1352.5 to 1365.0 cm^{-1} .

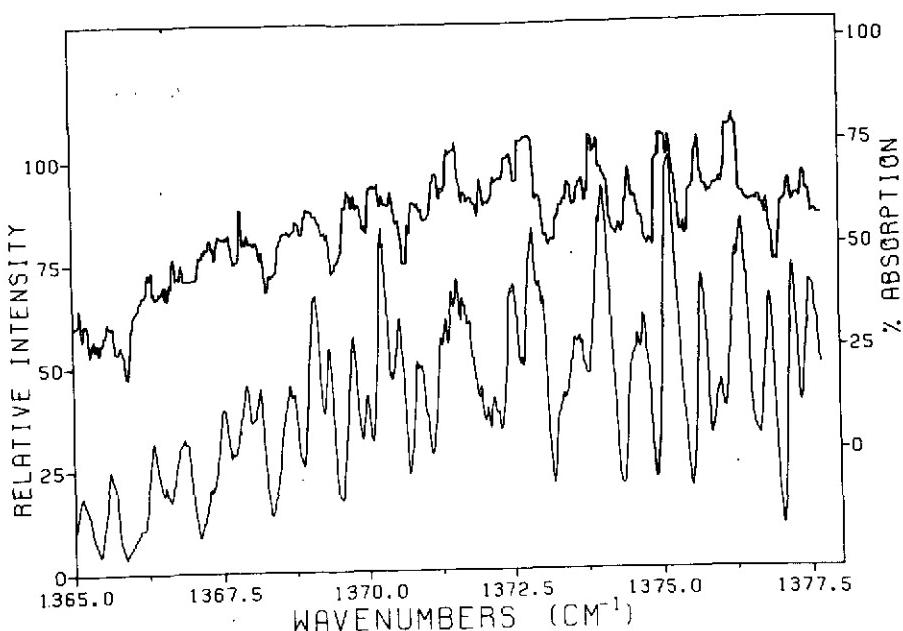


Fig. 3(d). Experimental and theoretical spectra of v_3 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1365.0 to 1377.5 cm^{-1} .

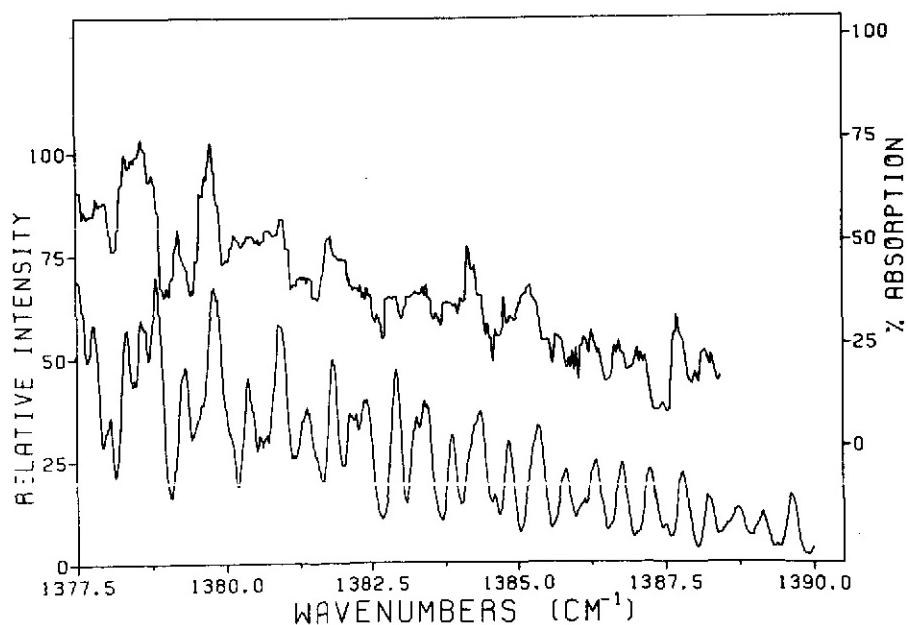


Fig. 3(e). Experimental and theoretical spectra of v_3 band of $^{32}\text{S}^{16}\text{O}_2$ in range 1377.5 to 1390.0 cm^{-1} .

TABLE V

COMPARISON OF EXPERIMENTAL AND THEORETICAL SPECTRAL LINE POSITIONS, WITH QUANTUM

NUMBER ASSIGNMENTS, FOR THE v_3 BAND OF $^{32}\text{S}^{16}\text{O}_2$ CENTERED AT $1362.00 \pm 0.10 \text{ cm}^{-1}$.

LINE INTENSITIES [SEE SEC. III, ESPECIALLY EQ. (6)] ARE COMPUTED AT 300°K.

Line Position (in cm^{-1})		Quantum Numbers								Line Position (in cm^{-1})		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$		
1327.57	1327.54	48	5	44	49	5	45	0.8793	1336.44	1336.43	38	2	37	39	2	38	3.6085		
1327.73	1327.70	44	13	32	45	13	33	0.4210	1336.51	1336.52	35	7	28	36	7	29	2.9345		
1327.87	1327.85	46	9	38	47	9	39	0.7091	1336.63	1336.63	33	11	22	34	11	23	1.7868		
	1327.88	45	11	34	46	11	35	0.5683	1336.73	1336.73	30	15	16	31	15	17	0.8060		
1328.05	1328.08	42	15	28	43	15	29	0.3207	1337.00	1336.99	34	8	27	35	8	28	2.7830		
1328.16	1328.13	46	8	39	47	8	40	0.8186	1337.08	1337.10	37	1	36	38	1	37	3.9428		
	1328.16	48	4	45	49	4	46	0.9741	1337.37	1337.35	32	11	22	33	11	23	1.9121		
1328.18	1328.18	44	12	33	45	12	34	0.5234	1337.46	1337.46	34	6	29	35	6	30	3.5706		
1328.55	1328.60	46	6	41	47	6	42	1.0321	1337.64	1337.65	34	5	30	35	5	31	3.9321		
1328.97	1328.92	45	5	40	46	5	41	1.2401	1337.76	1337.75	32	10	23	33	10	24	2.3199		
	1328.99	46	5	42	47	5	43	1.1368		1337.77	36	2	35	37	2	36	4.2919		
1329.01	1329.01	45	6	39	46	6	40	1.1571	1338.02	1338.01	29	14	15	30	14	16	1.1119		
1329.31	1329.35	45	4	41	46	4	42	1.3131	1338.08	1338.06	33	4	29	34	4	30	4.5280		
1329.73	1329.75	43	10	33	44	10	34	0.8590	1338.17	1338.16	33	6	27	34	6	28	3.8584		
1329.88	1329.86	44	7	38	45	7	39	1.1832		1338.19	33	5	28	34	5	29	4.2371		
1330.08	1330.09	44	6	39	45	6	40	1.3180	1338.47	1338.47	34	3	32	35	3	33	4.6191		
	1330.10	42	11	32	43	11	33	0.7988	1338.90	1338.91	32	6	27	33	6	28	4.1551		
1330.65	1330.64	40	13	28	41	13	29	0.6436	1339.09	1339.09	32	5	28	33	5	29	4.5825		
1330.93	1330.93	45	2	43	46	2	44	1.5717		1339.12	34	2	33	35	2	34	5.0326		
	1330.97	44	4	41	45	4	42	1.5919	1339.63	1339.62	31	6	25	32	6	26	4.4531		
1331.10	1331.12	42	8	35	43	8	36	1.3094	1340.12	1340.11	26	14	13	27	14	14	1.2229		
1331.25	1331.23	41	10	31	42	10	32	1.0671		1340.13	30	7	24	31	7	25	4.2197		
1331.37	1331.36	42	7	36	43	7	37	1.4874	1340.25	1340.25	29	9	20	30	9	21	3.3197		
1331.49	1331.53	43	3	40	44	3	41	1.7931	1340.34	1340.33	31	2	29	32	2	30	5.7889		
1331.61	1331.63	44	3	42	45	3	43	1.7629		1340.35	30	6	25	31	6	26	4.7537		
1331.73	1331.71	46	1	46	47	1	47	1.7901	1341.35	1341.34	25	13	12	26	13	13	1.6383		
1331.93	1331.96	40	10	31	41	10	32	1.1824	1341.64	1341.63	29	2	27	30	2	28	6.5907		
1332.35	1332.37	42	4	39	43	4	40	1.9947		1341.66	27	9	18	28	9	19	3.6629		
1332.56	1332.58	38	12	27	39	12	28	0.9705	1341.78	1341.77	30	2	29	31	2	30	6.6203		
1333.02	1333.01	42	3	40	43	3	41	2.1971		1341.79	31	0	31	32	0	32	6.7894		
	1333.03	43	1	42	44	1	43	2.2019	1342.29	1342.26	27	7	20	28	7	21	4.9739		
1333.05	40	6	35	41	6	36	2.0564		1342.28	25	11	14	26	11	15	2.6588			
1333.34	1333.32	40	5	36	41	5	37	2.2595	1342.48	1342.45	30	1	30	31	1	31	7.2104		
	1333.34	39	8	31	40	8	32	1.7895		1342.48	27	6	21	28	6	22	5.6251		
1333.69	1333.67	41	2	39	42	2	40	2.4422		1342.51	27	3	24	28	3	25	7.1054		
	1333.72	42	2	41	43	2	42	2.4470	1342.75	1342.73	23	13	10	24	13	11	1.6674		
1334.13	1334.15	37	10	27	38	10	28	1.5709	1342.99	1342.96	26	7	20	27	7	21	5.2037		
1334.29	1334.32	38	7	32	39	7	33	2.2456		1342.98	24	11	14	25	11	15	2.7207		
1334.40	1334.39	40	3	38	41	3	39	2.7015	1343.51	1343.56	26	4	23	27	4	24	7.1252		
	1334.40	41	1	40	42	1	41	2.7105	1344.05	1344.06	25	5	20	26	5	21	6.8310		
1334.55	1334.53	38	6	33	39	6	34	2.5108		1344.07	25	4	21	26	4	22	7.4217		
1334.83	1334.81	37	8	29	38	8	30	2.1613	1345.15	1345.15	22	9	14	23	9	15	4.2448		
1335.05	1335.03	39	2	37	40	2	38	2.9837	1345.27	1345.23	24	3	22	25	3	23	8.3171		
	1335.05	37	7	30	38	7	31	2.4647		1345.29	20	12	9	21	12	10	2.1121		
1335.08	37	4	33	38	4	34	3.1847		1345.30	23	6	17	24	6	18	6.5790			
1335.56	1335.54	36	8	29	37	8	30	2.3610	1345.95	1345.97	19	12	7	20	12	8	2.0396		
	1335.57	37	3	34	38	3	35	3.3480	1346.19	1346.16	21	8	13	22	8	14	5.1343		
1335.74	1335.76	39	1	38	40	1	39	3.2917		1346.19	22	5	18	23	5	19	7.5469		
1335.84	1335.80	40	1	40	41	1	41	3.3496	1346.26	1346.25	23	1	22	24	1	23	9.2116		
1336.28	1336.26	35	8	27	36	8	28	2.5686	1346.60	1346.58	22	3	20	23	3	21	8.8762		
	1336.32	34	10	25	35	10	26	2.0109	1346.99	1346.95	21	2	19	22	2	20	9.3946		

TABLE V (Continued)

Line Position (in cm^{-1})		Quantum Numbers								Line Position (in cm^{-1})		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$	Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o}{C'}$		
	1346.97	23	0	23	24	0	24	9.8178	1354.50	1354.52	19	19	0	19	19	1	1.0675		
	1347.01	22	2	21	23	2	22	9.4455	1354.60	1354.55	10	4	7	11	4	8	6.7871		
1347.18	1347.14	20	7	14	21	7	15	6.0759	1354.89	1354.92	8	8	1	9	8	2	2.8625		
	1347.21	19	9	10	20	9	11	4.2616	1355.25	1355.24	19	18	1	19	18	2	0.9670		
1347.30	1347.34	17	12	5	18	12	6	1.7973	1355.34	1355.30	9	1	8	10	1	9	8.1799		
1347.38	1347.38	20	6	15	21	6	16	6.9817	1355.75	1355.73	23	17	6	23	17	7	0.9836		
1347.49	1347.52	18	10	9	19	10	10	3.3407	1355.99	1355.99	8	3	6	9	3	7	6.4307		
	1347.52	21	1	20	22	1	21	9.7377	1356.09	1356.12	8	2	7	9	2	8	7.1660		
1347.59	1347.58	20	5	16	21	5	17	7.8440	1356.36	1356.34	7	5	2	8	5	3	3.5348		
	1347.62	22	1	22	23	1	23	10.0823	1356.42	1356.42	8	1	8	9	1	9	7.6733		
1347.72	1347.74	20	4	17	21	4	18	8.6200	1356.62	1356.61	18	16	3	18	16	2	2.0022		
1347.91	1347.89	18	9	10	19	9	11	4.1884		1356.64	7	1	6	8	1	7	6.9194		
	1347.93	20	3	18	21	3	19	9.2815		1356.64	7	3	4	8	3	5	5.6838		
1348.09	1348.07	19	6	13	20	6	14	7.0311		1356.79	1356.78	6	6	1	7	6	2	1.2615	
1348.31	1348.31	20	2	19	21	2	20	9.8640		1356.86	1356.87	25	15	10	25	15	11	1.0266	
	1348.32	19	2	17	20	2	18	9.7829		1357.02	1357.00	6	5	2	7	5	3	2.5490	
1348.86	1348.89	20	1	20	21	1	21	10.4854		1357.23	1357.22	18	15	4	18	15	3	2.2695	
1348.95	1348.96	18	5	14	19	5	15	7.9514		1357.26	1357.26	17	15	2	17	15	3	2.5354	
1349.15	1349.12	18	4	15	19	4	16	8.7841		1357.35	1357.33	15	15	0	15	15	1	3.1678	
	1349.14	15	11	4	16	11	5	2.0407		1358.05	1358.03	5	2	3	6	2	4	4.8131	
1349.35	1349.36	14	12	3	15	12	4	1.1363		1358.20	1358.18	5	0	5	6	0	6	5.5900	
1349.50	1349.51	19	0	19	20	0	20	10.6170		1358.22	1358.22	20	13	8	20	13	7	2.1608	
1349.69	1349.71	17	2	15	18	2	16	9.9530		1358.29	1358.27	19	13	6	19	13	7	2.4155	
1349.81	1349.78	17	3	14	18	3	15	9.4805		1358.31	1358.31	18	13	6	18	13	5	2.6989	
	1349.81	14	11	4	15	11	5	1.7620		1358.50	1358.49	13	13	0	13	13	1	4.7290	
1349.94	1349.92	15	9	6	16	9	7	3.6733		1358.83	1358.84	17	12	5	17	12	6	3.1241	
1350.05	1350.06	17	1	16	18	1	17	10.2536		1358.85	1358.85	26	11	16	26	11	15	1.1498	
1350.15	1350.12	16	6	11	17	6	12	6.8587		1358.94	1358.95	14	12	3	14	12	2	4.4117	
	1350.16	18	1	18	19	1	19	10.6817		1359.12	1359.12	21	11	10	21	11	11	2.0498	
1350.26	1350.23	14	10	5	15	10	6	2.5161		1359.23	1359.21	19	11	8	19	11	9	2.5636	
	1350.26	15	8	7	16	8	8	4.6333		1359.43	1359.40	14	11	4	14	11	3	4.4770	
1350.36	1350.33	16	5	12	17	5	13	7.8310		1359.43	1359.43	13	11	2	13	11	3	5.0204	
1350.48	1350.49	16	4	13	17	4	14	8.7144		1359.92	1359.90	11	10	1	11	10	2	6.2507	
1350.63	1350.60	14	9	6	15	9	7	3.3877		1359.92	1359.92	10	10	1	10	10	0	7.0834	
	1350.64	16	3	14	17	3	15	9.4630		1360.04	1360.03	18	9	12	20	9	11	2.1295	
1351.00	1351.00	15	5	10	16	5	11	7.6742		1360.27	1360.27	11	9	2	11	9	3	5.9171	
1351.11	1351.11	15	2	13	16	2	14	9.8638		1360.29	1360.29	10	9	2	10	9	1	6.7055	
1351.21	1351.20	15	3	12	16	3	13	9.3354		1360.35	1360.36	18	8	11	18	8	10	2.4157	
	1351.22	14	7	8	15	7	9	5.3836		1360.84	1360.84	13	7	6	13	7	7	3.6683	
1351.94	1351.94	12	9	4	13	9	5	2.6131		1361.06	1361.06	14	6	9	14	6	8	2.6706	
1352.19	1352.15	13	6	7	14	6	8	6.1112		1361.45	1361.45	7	5	2	7	5	3	5.0069	
	1352.22	14	2	13	15	2	14	9.7916		1361.46	1361.46	6	5	2	6	5	1	5.8958	
1352.37	1352.35	13	5	8	14	5	9	7.1475		1362.20	1362.18	9	2	7	9	2	8	0.6800	
1352.53	1352.51	13	2	11	14	2	12	9.4830		1362.64	1362.64	1	0	1	0	0	0	0.9982	
	1352.56	12	7	6	13	7	7	4.6334		1363.89	1363.89	3	0	3	2	0	2	2.9686	
1352.63	1352.60	13	3	10	14	3	11	8.9012		1363.99	1363.96	3	1	2	2	1	1	2.6174	
	1352.65	13	1	12	14	1	13	9.8033		1364.49	1364.45	4	2	3	3	2	2	2.8490	
1352.96	1352.94	11	8	3	12	8	4	3.0805		1364.83	1364.85	5	4	1	4	4	0	1.5310	
1353.17	1353.19	12	4	9	13	4	10	7.7425		1365.15	1365.13	5	0	5	4	0	4	4.8434	
1353.25	1353.23	13	0	13	14	0	14	10.1011		1365.24	1365.26	5	1	4	4	1	3	4.6113	
	1353.27	10	9	2	11	9	3	1.5169		1365.60	1365.60	6	1	6	5	1	5	5.5369	
1353.59	1353.60	10	8	3	11	8	4	2.4852		1365.69	1365.70	6	2	5	5	2	4	4.9313	
1353.68	1353.69	11	5	6	12	5	7	6.3101		1366.27	1366.24	7	3	4	6	3	3	4.9816	
1353.91	1353.89	10	7	4	11	7	5	3.5504		1366.36	1366.34	7	0	7	6	0	6	6.5562	
	1353.91	11	2	9	12	2	10	8.7906		1366.56	1366.54	7	1	6	6	1	5	6.3656	
1353.93	1353.93	12	1	12	13	1	13	9.7348		1366.72	1366.72	8	4	5	7	4	4	4.8364	
1353.98	1353.97	11	1	10	12	1	11	9.1436		1366.72	1366.72	8	4	5	7	4	4		
1354.23	1354.26	9	8	1	10	8	2	1.7865		1366.72	1366.69	9	7	2	8	7	1	2.1342	
1354.35	1354.36	10	5	6	11	5	7	5.7641		1366.72	1366.72	8	4	5	7	4	4		

TABLE V (Continued)

Line Position (in cm^{-1})		Quantum Numbers								Line Position (in cm^{-1})		Quantum Numbers							
Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^{\circ}}{C'}$	Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^{\circ}}{C'}$		
1366.87	1366.86	8	3	6	7	3	5	5.8689			1376.25	24	5	20	23	5	19	8.0821	
1367.36	1367.34	9	4	5	8	4	4	5.6831	1376.81	1376.82	25	1	24	24	1	23	9.8080		
1367.64	1367.67	9	2	7	8	2	6	7.4212	1377.19	1377.18	26	6	21	25	6	20	6.8219		
1367.85	1367.81	9	1	8	8	1	7	7.8726			1377.20	25	4	21	24	4	20	8.5470	
1367.95	1367.94	10	1	10	9	1	9	8.6178			1377.22	26	2	25	25	2	24	9.4444	
	1367.96	10	4	7	9	4	6	6.4331	1377.42	1377.42	28	9	20	27	9	19	4.0979		
1368.12	1368.15	10	2	9	9	2	8	8.1114			1377.43	26	5	22	25	5	21	7.5853	
1368.21	1368.24	12	8	5	11	8	4	3.2321	1377.63	1377.61	25	3	22	24	3	21	9.0766		
1368.65	1368.65	11	0	11	10	0	10	9.3010	1377.83	1377.84	27	1	26	26	1	25	9.1025		
1368.81	1368.79	12	6	7	11	6	6	5.4902	1378.31	1378.31	29	0	29	28	0	28	8.9600		
	1368.85	13	8	5	12	8	4	3.7762			1378.34	29	8	21	28	8	20	4.6134	
1369.29	1369.33	12	3	10	11	3	9	8.5616	1378.44	1378.46	27	4	23	26	4	22	7.9100		
1369.37	1369.35	12	2	11	11	2	10	9.2530	1378.60	1378.57	30	9	22	29	9	21	3.7439		
	1369.40	13	6	7	12	6	6	6.0186			1378.61	28	5	24	27	5	23	6.9791	
1369.73	1369.73	15	9	6	14	9	5	3.5974	1378.79	1378.76	28	4	25	27	4	24	7.5913		
	1369.76	13	0	13	12	0	12	10.2737	1379.03	1379.03	33	12	21	32	12	20	1.7647		
1369.84	1369.80	13	4	9	12	4	8	8.1565	1379.20	1379.23	30	7	24	29	7	23	5.0511		
	1369.82	18	13	6	17	13	5	1.3549	1379.58	1379.58	29	2	27	28	2	26	7.8515		
1370.00	1369.99	13	3	10	12	3	9	9.0279	1379.66	1379.66	35	13	22	34	13	21	1.2346		
	1370.01	14	6	9	13	6	8	6.4635	1379.77	1379.73	30	3	28	29	3	27	7.3461		
1370.22	1370.22	14	1	14	13	1	13	10.6174			1379.78	30	5	26	29	5	25	6.3026	
	1370.26	13	1	12	12	1	11	10.0292			1379.81	31	7	24	30	7	23	4.7786	
1370.31	1370.31	18	12	7	17	12	6	1.9317	1380.01	1380.01	29	3	26	28	3	25	7.5615		
	1370.33	16	9	8	15	9	7	3.9163	1380.14	1380.12	31	6	25	30	6	24	5.3833		
1370.43	1370.41	14	4	11	13	4	10	8.5657	1380.37	1380.35	32	2	31	31	2	30	7.0310		
1370.57	1370.55	14	3	12	13	3	11	9.4218			1380.37	33	0	33	32	0	32	7.2039	
1370.70	1370.67	16	8	9	15	8	8	4.9398	1380.55	1380.57	31	2	29	30	2	28	6.9989		
1370.88	1370.85	15	0	15	14	0	14	10.9608	1381.16	1381.15	31	3	28	30	3	27	6.7141		
	1370.90	19	12	7	18	12	6	2.0889	1381.33	1381.36	34	2	33	33	2	32	6.1753		
1370.98	1370.96	16	7	10	15	7	9	6.0231	1381.82	1381.83	34	3	32	33	3	31	5.7009		
1371.31	1371.34	16	1	16	15	1	15	11.1751	1382.31	1382.34	36	8	29	35	8	28	2.9679		
1371.44	1371.44	15	1	14	14	1	13	10.6475	1382.42	1382.40	37	0	37	36	0	36	5.4550		
	1371.44	16	5	12	15	5	11	8.1824	1382.58	1382.54	37	9	28	36	9	27	2.3546		
1371.55	1371.54	15	2	13	14	2	12	10.3274	1383.36	1383.39	39	0	39	38	0	38	4.6460		
1371.68	1371.67	22	14	9	21	14	8	1.3021	1383.44	1383.44	35	4	31	34	4	30	4.8160		
	1371.69	16	2	15	15	2	14	10.6161	1383.60	1383.63	37	6	31	36	6	30	3.4994		
1371.98	1371.94	17	0	17	16	0	16	11.3605	1383.94	1383.94	41	11	30	40	11	29	1.1589		
	1371.95	20	11	10	19	11	9	2.9085	1384.03	1384.03	39	8	31	38	8	30	2.3047		
1372.18	1372.16	18	7	12	17	7	11	6.4341	1384.14	1384.13	38	6	33	37	6	32	3.2140		
1372.47	1372.44	18	1	18	17	1	17	11.4436			1384.17	37	5	32	36	5	31	3.8266	
	1372.47	19	8	11	18	8	10	5.5112	1384.24	1384.22	38	4	35	37	4	34	3.8372		
1372.78	1372.76	19	7	12	18	7	11	6.5472			1384.25	37	3	34	36	3	33	4.2622	
1372.97	1372.96	18	3	16	17	3	15	10.2187	1384.49	1384.49	42	11	32	41	11	31	1.0509		
1373.28	1373.26	19	5	14	18	5	13	8.5806	1384.61	1384.59	40	8	33	39	8	32	2.1014		
1373.70	1373.68	19	1	18	18	1	17	11.0036			1384.61	37	4	33	36	4	32	4.0726	
1373.85	1373.86	20	5	16	19	5	15	8.5855	1384.78	1384.77	41	9	32	40	9	31	1.6462		
1373.96	1373.96	20	2	19	19	2	18	10.8171			1384.81	39	6	33	38	6	32	2.9327	
1374.34	1374.30	24	11	14	23	11	13	3.0426	1385.86	1385.85	44	1	44	43	1	43	2.9281		
1374.49	1374.46	21	5	16	20	5	15	8.5330	1385.99	1386.00	41	6	35	40	6	34	2.4187		
1375.17	1375.14	23	7	16	22	7	15	6.4815	1386.27	1386.25	42	4	39	41	4	38	2.6238		
	1375.16	23	0	23	22	0	22	10.9944			1386.30	44	2	43	43	2	42	2.6030	
1375.42	1375.41	23	6	17	22	6	16	7.4030	1386.38	1386.37	42	6	37	41	6	36	2.1911		
	1375.43	24	8	17	23	8	16	5.4631	1386.64	1386.65	41	5	36	40	5	35	2.6254		
1375.66	1375.66	23	5	18	22	5	17	8.2759	1386.74	1386.78	45	1	44	44	1	43	2.3430		
	1375.68	24	1	24	23	1	23	10.7412	1387.02	1387.03	43	3	40	42	3	39	2.3802		
1376.03	1376.00	24	6	19	23	6	18	7.2437	1387.70	1387.73	47	1	46	46	1	45	1.8796		
1376.14	1376.15	24	2	23	23	2	22	10.0732	1388.03	1388.06	47	9	38	46	9	37	0.8565		
	1376.17	28	12	17	27	12	16	2.2261	1388.17	1388.20	46	4	43	45	4	42	1.6966		
1376.24	1376.22	25	0	25	24	0	24	10.4499	1388.29	1388.29	46	7	40	45	7	39	1.2628		

we have assigned only the approximately 250 observed peaks which are either individual or consist of a small number of closely spaced transitions. The band center for ν_3 in the present work has been determined as 1362.00 ± 0.10 cm^{-1} . Previously obtained values were 1361 (Ref. 26), 1361.50 (Ref. 27), 1361.76 (Ref. 1), 1360.5 ± 0.5 (Ref. 28), and 1360.8 cm^{-1} (Ref. 29).

Finally, we have estimated the absolute values of the dipole moment derivatives³¹ for all three infrared-active fundamentals of $^{32}\text{S}^{16}\text{O}_2$. Our analysis, using Eqs.(6) and (7), was described in detail in Sec. III. The results are shown in Table VI. The ν_1 band intensity of Hinkley *et al.*⁸ was an average of the projected values which were obtained by dividing the intensities of ten measured lines by their respective calculated fractional contributions to the band.

TABLE VI
DIPOLE MOMENT DERIVATIVES FOR THE FUNDAMENTALS OF $^{32}\text{S}^{16}\text{O}_2$

Band	Sum of Calculated Line Intensities (dimensionless)	Measured Band Intensity (in $10^{10} \text{ sec}^{-1} \text{ cm}^{-1}$ STP)	Dipole Moment Derivative ^f (in esu $\text{g}^{-1/2}$)
ν_1	5227.9	278 ± 28^a	57.8 ± 3.0
		317 ± 8^b	61.7 ± 0.8
		350 ± 20^c	64.8 ± 1.9
		288 ± 16^d	58.9 ± 1.7
		299 ± 16^e	59.9 ± 1.6
ν_2	5288.6	348 ± 35^a	64.3 ± 3.3
		376 ± 20^b	66.8 ± 1.8
		360 ± 30^c	65.4 ± 2.8
ν_3	5742.3	2520 ± 252^a	166.0 ± 9.0
		2560 ± 70^b	167.3 ± 2.3
		2640 ± 80^c	169.9 ± 2.6
		2437 ± 161^e	163.1 ± 5.5

^aFrom Ref. 20.

^bFrom Ref. 21.

^cFrom Ref. 22.

^dFrom Ref. 8.

^eFrom Ref. 23.

^fAs discussed in Sec. III, only the absolute value can be determined here.

V. DISCUSSION

There is considerable value, from a fundamental spectroscopic viewpoint, in making high-resolution studies of gases like SO_2 . Such studies would permit a more complete determination of vibration-rotation line positions and intensities, as well as quantum-number assignments, in all three fundamentals. Further, it would be possible to measure line-shapes and line-broadening parameters as a function of vibration and/or rotation quantum numbers. Some of these experimental and theoretical studies are in progress, and some are anticipated in our laboratory in the near future.

We also plan to investigate overtone and combination bands of SO_2 . A more precise determination of the band center of $2\nu_2$ is important to an understanding of possible lasing mechanisms³² in SO_2 , associated with Fermi interactions between energy levels in ν_1 and $2\nu_2$. In another context, it is possible that the $\nu_1 + \nu_3$ band of terrestrial SO_2 may appear in solar spectra,³³ and be susceptible to analysis there.

Sulfur dioxide plays a serious role as a pollutant in the terrestrial atmosphere.³⁴ High-resolution infrared spectroscopy is a possible technique for the remote detection and monitoring of SO_2 in situ. For example, monochromatic laser emissions may be useful for studying terrestrial SO_2 in absorption. We have found three relatively isolated and moderately strong lines in our laboratory spectra, with observed positions at 561.67, 1347.33, and 1365.60 cm^{-1} (see Tables IV and V) which fall close to observed laser oscillations³⁵ in pure neutral neon, Ne I. Although the spectral coincidences are not exact for the first two lines, nevertheless the spectral broadening by air will produce sufficient overlapping of the lines in question.³⁶

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